

# Adaptive numerical modelling and hybrid physically based ANM approaches in materials engineering – a survey

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Many adaptive numerical modelling (ANM) techniques such as artificial neural networks (including multilayer perceptrons), support vector machines and Gaussian processes have now been applied to a wide range of regression and classification problems in materials science. Materials science offers a wide range of industrial applications and hence problem complexity levels from well physically characterised systems (e.g. high value, low volume products) to high volume low cost applications with intrinsic scatter due to commercial manufacturing processes. The authors review a number of recent examples in the literature, with the aim of identifying best practice in the use of these techniques as part of a multistrand modelling approach. The importance of understanding the basic principles of these modelling techniques and how they can link with other modelling strategies is emphasised. In particular the authors wish to identify the importance of hybrid physically based ANM in taking the field forward, which can range from, at the most basic level, careful data selection and data preprocessing to a full integration of physically based models with advanced ANM. A number of case studies are presented to illustrate the main points of the paper.

**Keywords:** Neural networks, Support vector machines, Gaussian processes, Adaptive numerical modelling, Data driven techniques, Hybrid modelling, Applications in materials science

## Introduction

The links between processing variables, microstructure evolution, resultant properties and hence mechanical performance are core tenets of materials engineering and a variety of modelling approaches have been applied to these materials modelling challenges. In some cases, a clear physical basis for such models has now been established, but often these can apply only to well defined conditions, which may not be representative of either genuine industrial (scaled up) production processes, or materials performance under realistic service conditions. The advantages of physically based models are:

- (i) they are robust to interpolation and extrapolation (as long as the underlying physical mechanisms being modelled are in operation)
- (ii) they should not require large amounts of data, as typically they only have a limited number of fitted parameters; ideally, a physically based model may have no fitted parameters

- (iii) the mechanistic verifications derived from physically based modelling may also offer insights into novel materials optimisation strategies
- (iv) a physically based model is relatively transparent, i.e. the mathematical underlying relationships between input and output parameters may be written in a reasonably clear mathematical form: this is part of a loosely defined group of methods which the authors term ‘white box’.

However, in a truly integrated processing–performance model, with the levels of uncertainty and complexity associated with industrial practice and complex service conditions, expressing these interlinked processes purely on physics based principles is unlikely to be feasible. A white box model will require extensive further data set generation which may be too costly, but also not possible for the actual processes in production. In such circumstances empirically fitting relationships to the observed data has a useful role to play.

Such data driven approaches can be broadly classified into:

- (i) regression approaches, where a set of inputs give rise to a continuous output or outputs (i.e. a varying quantity or quantities) or
- (ii) classification, where the input data is used to define to which class the input data correlate.

Statistically based regression or classification approaches usually use defined functions as the mapping

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functions and the fittable parameters can be found by a variety of means. By whatever means a regression or classification fitting function is found, there are always important caveats to be observed when comparing interpolation (working within the input space) where the model function is likely to be well defined and extrapolation, where little or no data exists to guide the model, and indeed where different mechanisms or regimes of behaviour may come into play.

In the field of machine learning, a wide range of sophisticated adaptive numerical modelling (ANM) approaches have been developed in the fields of regression and classification, including: fuzzy logic, neural networks, support vector machines, genetic algorithms, Gaussian processes and Bayesian methods, etc. In the authors' terminology, an adaptive numerical model effectively searches parameter and function space in finding a solution, which can also be considered to be an optimisation problem, so the basis of all these approaches is the fitting of a suitable flexible function to a set of input parameters to generate a prediction of an output set (which may be a class definition). The function is progressively refined (by adaptive or optimisation processes – a large research area in its own right) by comparison of the predicted output with the target output (i.e. known output values, for these input values). This is usually achieved by minimising an objective function that measures the closeness of fit between prediction and target. The general requirements for employing such approaches are:

- (i) the input data set describe the problem adequately, over the appropriate data input ranges
- (ii) there are sufficient data, well distributed across the multidimensional input space, to determine the function parameters
- (iii) the problem should be well posed, in that the solution (e.g. minimisation of the objective function) can be uniquely identified
- (iv) an appropriate general fitting function or function set is used.

It can be seen that identifying the input set and function type requires a degree of mechanistic (physics based) insight, so these are never purely data driven approaches. The potential for exploiting a combination of such data derived models with appropriate functions based on mechanistic insight is very exciting, particularly for the integrated multiscale models which are now required for industrial applications of materials engineering. Such hybrid physically based ANM approaches can also offer important insights into probabilistic modelling (where the effect of levels of uncertainty in processing or service conditions) can be assessed. The present paper aims to review recent work in this field within materials science, starting with a brief recap on the conceptual basis of several regression and classification approaches, and then comparison of recent published work with specific case studies drawn from work at Southampton University exemplifying the advantages and drawbacks of some of these approaches.

## Conceptual basis of adaptive numerical modelling

Many adaptive numerical modelling approaches have been developed for regression and classification

purposes, including: multilayer perceptrons (MLPs, also termed artificial neural networks (ANNs)) fuzzy logic, support vector machines (SVM), Gaussian processes, Bayesian methods and response surfaces, etc. As mentioned previously, the basis of many of these approaches is the fitting of a suitable flexible (multi-parameter) function to a set of input parameters to generate a prediction of an output set (which may be a class definition). The function is then progressively refined by comparison of the predicted output with the target output (i.e. known output values, for these input values). This is usually achieved by minimising an objective function (often the mean squared error (MSE) or its root) that measures the closeness of fit between prediction and target.

As may be seen in the following review, some papers in the materials field do not always clearly specify the techniques used, often appearing to use particularly ANNs as a true 'black box' system. This may lead to misleading findings (for instance in the form of oversimplified or trivial models) if there is insufficient understanding of the possible drawbacks and limitations of these approaches so that the results are not always critically reviewed. At the very least the authors propose that ANM predictions need to be assessed against either materials science knowledge, another physically based model or other differing regression techniques (the simplest of which may be a multiple linear regression technique). Presenting the results of a single ANM approach without benchmarking against other techniques may be a major stumbling block to the wider acceptance of the use of such techniques within the materials community.

Broadly, adaptive numeric modelling may be defined as follows; given some data with input  $n$ -dimensional  $\mathbf{x}$  and output  $y$

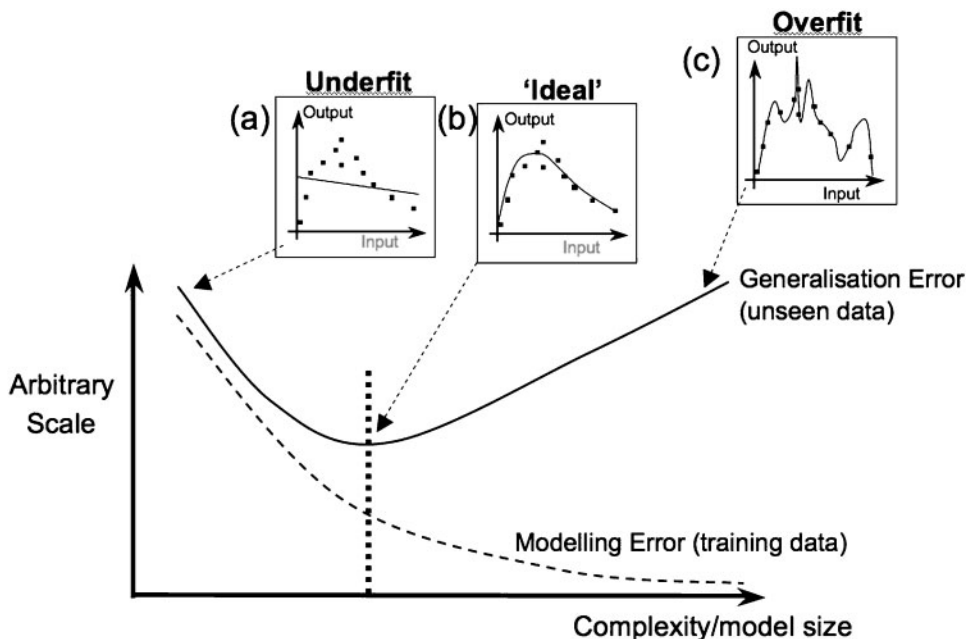
$$(y_1, \mathbf{x}_1), \dots, (y_l, \mathbf{x}_l), \mathbf{x} \in R^n, y \in R \quad (1)$$

the authors choose a model,  $m$ , from some set

$$M = \{m | m : R^n \rightarrow R\} \quad (2)$$

such that  $m$  approximates the data, and generalises well to new, unobserved data.

One key requirement in using such ANM techniques convincingly has been to assess generalisation performance, i.e. to examine model predictions on new or unseen 'test' data, which have not been used to define the fitting parameters in the model (as of course the original training data has been). Problems associated with generalisation can be seen in Fig. 1, where a schematic representation of how training error and test error vary with increasing model size/complexity can be seen. An overly simple linear model (Fig. 1a) underfits the training data but is relatively insensitive (or robust) to which training data are used to define the model. Figure 1c shows a typical overfit to the training data, where the function defined is highly sensitive to the choice of training data, and gives higher test errors comparing with the intermediate case (Fig. 1b) where the best generalisation performance can be seen. These underlying principles are well established in the ANM field and can be broadly described as the bias/variance trade-off, but as will be seen in this review, it is not always clear that these basic checks have been carried out when reporting predictive 'successes'.



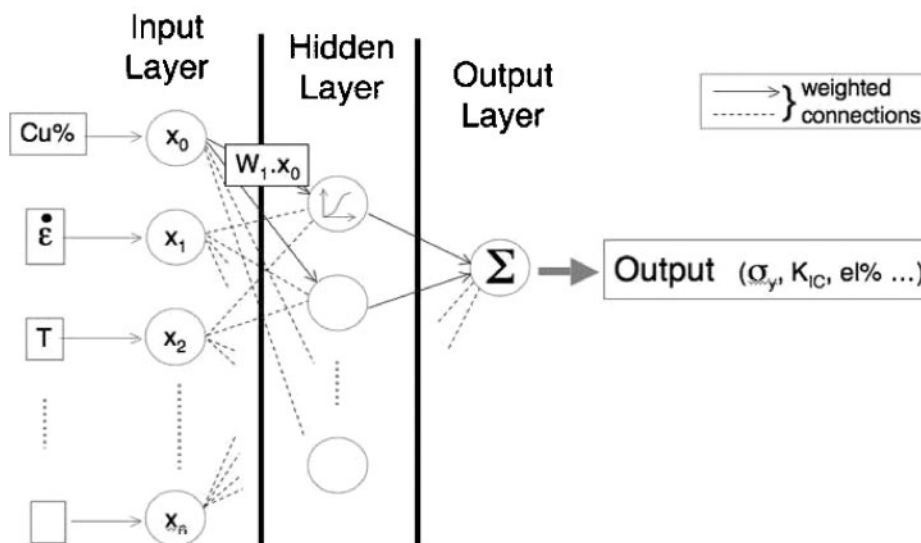
1 Comparison of training and test (unseen) error with increasing model complexity

**Description of specific ANM techniques**

*Artificial neural networks and multilayer perceptrons*

Artificial neural networks are often identified as multi-layer perceptrons, MLPs, although strictly speaking these are a subset of ANNs and are probably the most widely used ANM approach.<sup>1</sup> The network consists of many simple interconnected nodes with weighted connections, and these weights can be adapted on the basis of the training data presented to the network. These adaptations are based on a number of techniques that have arisen from regression analysis, statistical inferencing, machine learning and computational learning theory. There is a wide range of ANN algorithms used, many of which are trained using a supervised learning paradigm to generate the weight values. A typical MLP is illustrated in Fig. 2, and here the weights are adjusted on the interconnections between the input and output layers of nodes. Each node represents a function where the node output is a non-linear (often sigmoidal)

mapping of the input or sum of the inputs. Learning (or training) of the network proceeds by adjustment of the weights in the light of comparison with the predicted and actual (or target) output. The choice of model architecture (particularly the number of nodes and connections to and from the hidden layer) controls the complexity of the fitting function, but this same complexity may prevent direct representation of the underlying trends between input and output parameters (leading to the term ‘black box’ modelling sometimes being attributed to these approaches). The tendency to underfit or overfit a problem is then most simply controlled by increasing or decreasing the number of nodes in the hidden layer. So typical use of a MLP requires that an appropriate model architecture be defined often by an iterative procedure, which may or may not be defined automatically within the modelling package used. Another model initialisation issue is the choice of initial starting weights used on the interconnections, from which the model will start its progressive



2 Typical MLP architecture

refinements to fit to the training data supplied. There is a possibility that a local minimum in the MSE prediction (between target and prediction) may be found (rather than the global minimum in the objective function), depending on the starting point. A further important model initialisation issue is the split into test and train data, if this is carried out randomly each time a model is developed, the difference between the test and train data set splits may give rise to different final optimised models. Typically therefore a number of different model architectures, with differing weighted connections, may give quite similar predictive success. This has led to the use of model committees, where the averaged prediction from a number of similarly performing models may be used. Consideration of whether individual data points may then be exercising 'undue' influence (e.g. having been sampled more than is representative) on a final prediction is then often obscured.<sup>2</sup> Many current MLP packages make automatic choices in searching model space, in terms of the range of starting weights and model architectures examined, etc., and it is important that users of these packages appreciate the importance of such choices (which may no longer be under their control, as MLPs are now offered as a standard modelling technique in many commercial software packages e.g. Neural Toolbox within MATLAB). Some MLPs can however offer a degree of model insight with automatic relevance determination parameters being associated with certain inputs.

#### Bayesian frameworks in MLPs

Another important technique development is the use of Bayesian frameworks in MLPs (which essentially establish a probability distribution for the input data set that is progressively refined during training) thus allowing an error band to be defined for any predictions, basically reflecting the amount of knowledge the model has in that area of input space. The use of Bayesian frameworks in MLPs has therefore been the subject of significant interest in the materials modelling field.<sup>3</sup> These allow the probability of a model being a true representation of the data to be assessed, through an explicit representation of the model's inherent parametric uncertainty due to the limited dataset. A Bayesian MLP encompasses all of the key features of the classical MLP, but differs in that network training takes place using Bayesian learning. The result of Bayesian learning is a probability distribution over model parameters that expresses how likely the different parameter values are. This is advantageous since it allows the uncertainty of model predictions to be quantified via error bars. Initially, a wide prior distribution is defined which might express some rather general properties such as smoothness of the network function, but will otherwise leave the weight values fairly unconstrained. Upon observation of the data, this wide prior distribution is converted to a posterior distribution using Bayes' theorem

$$P(B|A) = \frac{P(A|B)P(B)}{P(A)} \quad (3)$$

where  $P(B|A)$  is the posterior distribution,  $P(A|B)$  is the likelihood function and  $P(B)$  is the prior distribution. The posterior distribution will be more compact, expressing the fact that the authors have learned

something about the extent to which different weight values are consistent with the observed data as the model trains. Thus each network also calculates a statistical 'error bar' for each point it predicts. This is not an experimental error, but is a measure of how confident the model is of the prediction, and allows for this inherent parametric uncertainty. The error bar typically represents a confidence of one standard deviation, or 67% and, as mentioned before, is useful in indicating where the MLP may have little training data to define its prediction. A Gaussian process can be used as a prior probability distribution over functions in Bayesian inference.

#### Genetic algorithms

Genetic algorithms (GAs) are biologically inspired computing techniques, which tend to mimic the basic Darwinian concepts of natural selection, and a review of their application to the materials science domain has been made by Chakraborti.<sup>4</sup> Candidate solutions (sometimes called individuals or creatures) to an optimisation or regression problem 'evolve' toward better solutions. This evolution usually starts from a population of randomly generated solutions and happens in generations. In each generation, the fitness (using an objective function as in other ANM techniques) of every solution is assessed, multiple solutions with the best 'fitness' are stochastically selected from the current population and modified (recombined and possibly randomly mutated) to form a new population. The new population is then used in the next iteration of the algorithm. The algorithm may terminate after either a specified fitness level is reached or a maximum number of generations has been produced (which may mean a satisfactory solution has not been reached). In many problems, GAs may also have a tendency to converge towards local optima in the objective function or even arbitrary points rather than the global optimum of the problem. Hence GAs are an optimisation tool, which can be used in converging upon a solution (or model).

#### Fuzzy logic and neurofuzzy modelling

Fuzzy logic is used to represent imprecise knowledge, sometimes expert knowledge may be stated in naturalistic language. Fuzzy sets form the basis of fuzzy logic and they provide absolute mathematical interpretation to vague concepts.<sup>5,6</sup> In contrast to classical logic an element may be a partial member of a fuzzy set, which allows a gradual transition between membership and non-membership whereas in classical logic an element must be wholly included or entirely excluded from a set. A fuzzy rule is of the form

$$\begin{aligned} r_{ij} : & \text{IF}(x_1 \text{ is } A_1^i \text{ AND } x_2 \text{ is } A_2^i \text{ AND } \dots \text{ AND } x_n \text{ is } A_n^i) \\ & \text{THEN}(y \text{ is } B_j) \end{aligned} \quad (4)$$

where  $x_k$  is the  $k$ th real valued input,  $y$  is the output,  $r_{ij}$  is the  $ij$ th fuzzy rule,  $A_k^i$  is the univariate linguistic term (or fuzzy set) and  $B_j$  is the corresponding output linguistic rule. For example, IF (temperature is high) AND (environment is corrosive) THEN (fatigue life is short). Associated with each rule is a rule confidence  $c_{ij}$ , which is a measure of the degree of the contribution of the rule to the output. A rule confidence of zero means that the rule does not contribute to the output, and a rule confidence of one means that the rule is completely true.

Neurofuzzy modelling<sup>7</sup> combines such qualitative, rule based representation of the derived model with the structural and learning abilities commonly associated with ANNs and can be thought of as an ANN that simplifies considerably the interconnectivity of the computational nodes, with the neurofuzzy submodels being connected directly to the input values. The development of the model structure is then based on an analysis of variables (ANOVA) representation to model the additive structural relationships that may exist in the data.

The ANOVA representation is the concept that any high dimensional function can be broken down into a subset of terms from the expansion

$$f(x) = f_0 + \sum_{i=1}^N f_i(x_i) + \sum_{i=1}^N \sum_{j=1+1}^N f_{i,j}(x_i, x_j) + \dots + f_{1,2 \dots N}(x) \quad (5)$$

where  $N$  represents the number of input parameters,  $f_0$  is a constant (bias term) and the other terms on the right hand side represent all possible univariate, bivariate and trivariate etc. functional combination of the input parameters (which in this case represent the neurofuzzy submodels). This then allows the network's output to be expressed as the smallest possible number of these neurofuzzy systems (or 'subnetworks'), each with a limited number of inputs from the main input vector. This simplified additive network reduces the resources (quantity of data) required to implement a robust fuzzy system (compared with having one large network taking all the input variables), and gives improved generalisation ability, while also increasing the transparency of the network by simplifying the linguistic fuzzy rules produced. A one step ahead iterative error minimisation technique builds up the models incrementally by systematically testing a range of model changes and incorporating the most statistically significant ones. In summary, such neurofuzzy algorithms combine pure neural network empirical data modelling techniques with a fuzzy logic based representation. This can allow rules to be used to initialise the network (define sensible starting points) and also to verify relationships extracted from the data by the network against physical understanding, thus providing a degree of model transparency.

#### Support vector machines

Support vector machines have a strong theoretical foundation and promising empirical performance. The initial development of SVMs was driven by attempts to resolve the bias/variance trade-off (as mentioned earlier), model complexity issues and the incidence of model overfitting. This formulation embodies the principle of structural risk minimisation developed by Vapnik.<sup>8</sup> Support vector machines make use of reproducing kernels which are functions that provide an elegant approach to dealing with non-linear algorithms by enabling computations to be carried out in the input space as opposed to the potentially high dimensional feature space. In work at Southampton<sup>9</sup> spline kernels have been used due to their ability to approximate arbitrary functions and a quadratic loss function is used (which gives a solution that is identical to the Gaussian process). Support vector machines, like MLPs, are however essentially black box models but transparency

can be introduced by the use of the Support vector Parsimonious ANOVA (SUPANOVA).<sup>10</sup> The SUPANOVA technique selects a small set of the most influential terms from the complete ANOVA representation (equation (5)) to provide a simple, global model representation. It is distinct from the neurofuzzy approach in that it first determines the full model before selecting the most significant ANOVA terms, avoiding the local minima trapping in MSE which can occur in the iterative model selection procedure used by the neurofuzzy method, GAs and some MLPs.

## Processing models

### Microstructure prediction models (including classification approaches)

A key approach in materials science is the successful prediction of microstructure evolution from processing conditions. There are a number of reports in the literature which have focussed on the ANM prediction of microstructure from processing conditions, most of which are regression approaches.

Predictions of porosity in NiTi shape memory alloy<sup>11</sup> and Al-Si casting alloys<sup>12</sup> have been reported where processing conditions (e.g. compaction pressure, sintering temperature and time, or chemical composition and cooling rate respectively) have been used as input parameters and predicted porosity. The criteria for successful predictions adopted in these papers may be considered limited however, as they do not include comparison of the apparent predictive success of their ANM approach with other regression methods (which might be developed for such processing microstructure datasets simply by inspection or classical statistical analysis), or interrogation of their models against physically based models/understanding.

A more interesting classification approach is reported by Al-Khedler *et al.*<sup>13</sup> where SEM based image analysis of carbon nanotube (CNT) structures has been developed to describe stereological relationships. This less intuitive input-output data set has then been assessed using an ANN classifier, which was also used to assess possible links between Raman spectra of CNTs and the quality of the resultant mass CNT structures. This would appear to be an effective use of the capabilities of ANM, with applications to quick and precise characterisation of a batch of CNTs (a barrier to successful mass production of these structures).

Other reported applications include regression modelling of mechanical alloying parameters (milling time and speed, ball to powder weight ratio) on crystallite size and lattice strain in Al-8 vol.-%SiC nanocomposites.<sup>14</sup> Here the authors have compared two different types of neural network architecture, MLPs and radial basis functions and have also presented the response surfaces between the input-output data set. The definition or control of the MLP structure (which had more nodes) may be the key to the reported improved predictive success of the MLP over the radial basis functions.

Adaptive numerical modelling assessments have also been reported on pearlite growth rate as a function of chemical composition<sup>15</sup> or strain induced transformation of retained austenite in transformation induced plasticity aided steels as a function of the driving force for martensitic transformation, initial retained austenite

content, matrix microstructure and forming conditions.<sup>16</sup> The latter paper has again used a physics based description (driving force for martensitic transformation) as an input which can be thought of as an input preselection, preprocessing or feature extraction process, where the input variables are manipulated into as relevant a form as possible in the light of metallurgical understanding – this can also be considered another way of incorporating physical understanding into use of ANMs, i.e. an avenue of hybridisation between physically based models and purely data driven techniques.

Precipitation behaviour has been assessed via an ANOVA in an adaptive numerical regression approach in commercial duplex stainless steels (assessing volume fractions of  $\sigma$  phase after annealing treatments) and 2219 Al alloys (assessing age hardening response during complex heat treatments)<sup>17</sup> for complex datasets from heat treatment trials under a range of commercial processing conditions, this enabled an estimate of the most influential parameters to be made. The age hardening behaviour of Al–Si–Mg alloys has also been studied<sup>18</sup> where the aging behaviour of AA6022 has been assessed by TEM based studies, using an image analysis algorithm which captured orientation gradient, nearest neighbour distances, number density, shapes and sizes of precipitates and their influence on hardness. A parametric study was first performed to identify the significance of each precipitate parameter, and then only the most important precipitate parameters (e.g. volume fraction, size, shape and inter precipitate distance) used to predict the hardening response.

Grain size prediction using ANNs has been attempted by a number of authors, e.g. in dynamic recrystallisation of austenitic stainless steels<sup>19</sup> and in the HAZ in a Ti6Al4V weldment.<sup>20</sup> In both these approaches processing parameters such as temperature and strain level or current and welding speed are used as inputs, and hence allow processing parameter microstructure maps to be developed. This also shows how classification of which processing parameters (e.g. operator controlled features) affect more directly relevant physical features (e.g. weld pool shape, temperature profile etc). This may be a useful interpolation step in such models to improve processing control. Sabin *et al.*<sup>21</sup> used Gaussian processes (within a Bayesian framework) to predict static recrystallisation in an Al–Mg alloy. This then allowed the certainty level (or noise) in their predictions to be shown. Sellars *et al.*<sup>22</sup> have perhaps shown a more sophisticated hybrid approach to grain size prediction using GAs to optimise the constants in their internal state variables for dislocation density, subgrain size and misorientation as the intermediate step in predicting flow stress and recrystallisation behaviour as a function of changing process histories in a range of Al–Mg alloys.

#### Case study

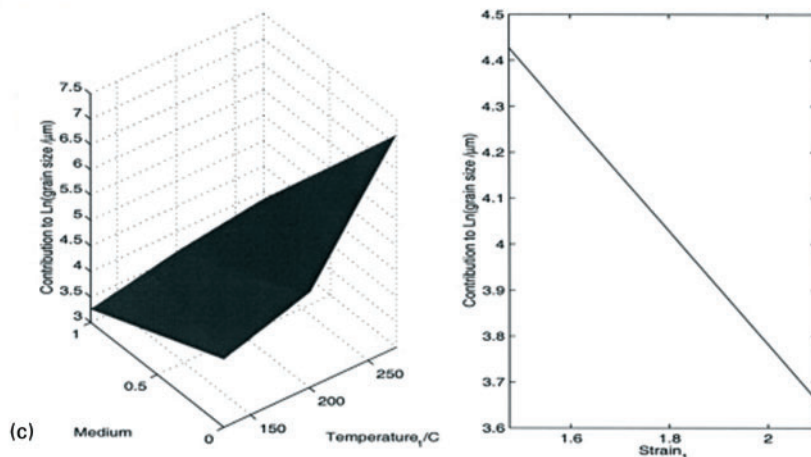
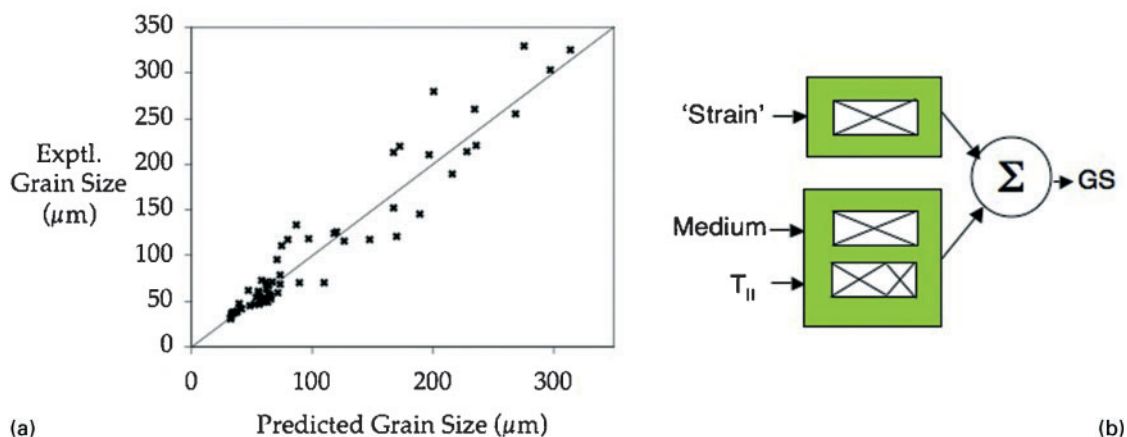
Clinch *et al.*<sup>23</sup> have illustrated how microstructure prediction can be carried out to predict final grain size in the ‘heading’ process applied to aluminium high pressure gas cylinders. Particularly, a form of hybrid modelling was required for what is in fact a reasonably simple metal forming operation (two deformation steps, two thermal treatments). Inputs were derived from direct physical parameters (such as temperature), finite element modelling (of the deformation process, leading to strain and strain rate parameters) and categorical

representation of equipment characteristics (oven type), along with materials properties at an intermediate state of the processing (hardness measured in between process steps to infer retained cold working strain). The neurofuzzy algorithm used in this instance employed an additive spline modelling on observational data approach, with forward selection/backwards elimination, allowing the algorithm to select and deselect inputs according to their statistical significance: as such data was presented to the model as a mixture of both ‘raw’ values, and physically informed transformations of input variables (e.g. logarithmic representation where power law relationships are expected), with the algorithm then being allowed to identify the most useful for the final model.

Given limited data availability in this instance test error had to be carried out via leave-one-out cross validation, with an equivalent benchmarking exercise being carried out against a multivariate linear regression (MLR). The validity of the modelling exercise was further checked in terms of the similarity in test and train errors (confirming reasonable generalisation), assessment against errors in original data gathering, and comparison of underlying relationships between inputs and outputs (explicitly produced by the ‘white box’ neurofuzzy approach) and physical understanding/expectation. Figure 3 illustrates typical model performance in terms of experimental versus predicted grain dimensions, along with an example model structure in terms of fuzzy rule base and associated functional relationships. It is via this combination of data representation, modelling selection, benchmarking and physical validation that a level of model confidence is achieved.

#### Prediction of hot deformation processes

The prediction of hot deformation processes may be considered a well developed subset of microstructure modelling. Modelling of hot deformation processing typically may involve constitutive relationships that relate different process variables to the flow stress of the deforming material, often by the use of internal state variables comprising an element of physical ‘meaning’ such as dislocation density, subgrain size, misorientation etc as described by Abbod *et al.*<sup>24</sup> They used data driven neurofuzzy models to derive the relationship between process history and the aforementioned internal state variables, then a physically based model to link the internal state variables to resultant flow stress and recrystallisation behaviour, finally using a GA approach to optimise the overall hybrid model constants to describe the hot deformation behaviour of a range of Al–Mg alloys. The same group has also applied a similar approach to modelling the flow behaviour, recrystallisation and crystallographic texture development in hot deformed Fe–30 wt-%Ni austenite<sup>25</sup> where they characterised grain structure, texture and dislocation substructure using EBSD and TEM approaches as a function of applied temperature and strain (as inputs). The compression flow stress was described as an empirically determined function of these inputs, whereas the recrystallisation behaviour was predicted by a physically based model from these measured microstructural internal state variables and texture was separately modelled using ANNs.



a experimental versus predicted grain dimensions; b example fuzzy rule base linking three inputs (representing deformation strain, quench medium and forming temperature); c corresponding bivariate and univariate functions contributing to (natural log of) grain size

### 3 Neurofuzzy modelling outcomes for cylinder heading process

A similar problem, predicting the flow stress of carbon steels, was used as an exemplar by Kumar *et al.*<sup>26</sup> for the expert systems community, where a recurrent self-organising neural network model was used (one that automatically adjusted its structure in view of its success in predicting data sets comparing with ANNs which typically have to have their architecture defined). This may be a somewhat misleading comparison as more sophisticated ANNs now exist in commercial modelling packages which also automatically alter, compare and combine ANN architectures to improve prediction.<sup>27</sup> It is important that the materials community recognise what these more sophisticated ‘prepackaged’ modelling approaches now offer, and the basis on which they select and combine models. Simply quoting test (or even training) errors as evidence of ‘good’ predictive modelling is insufficient/naïve.

#### Prediction of manufacturing processes

In considering manufacturing processes ANM approaches may be useful in correlating more easily controlled operating parameters to more physically significant parameters that control actual microstructure development. One example of this is the use by Vasudevan *et al.*<sup>28</sup> of GA models to optimise activated tungsten inert gas welding process parameters such as current, voltage, torch speed and arc gap on weld bead geometry (e.g. bead width, depth of penetration, etc.) in stainless steels. Another example is the use by Pagratis

*et al.*<sup>29</sup> of GA to link between several modelling stages. Process parameters were first determined by experimental validation of temperature versus time profiles for solid investment casting to calibrate the overall heat transfer coefficient at the metal mould interface to allow validated use of a commercial casting simulation. In addition the simulation was further interrogated by metallographic assessment of how microstructure and observed defects of the casting correlate with the simulation’s temperature distribution and porosity predictions and an ANN used to generate a predictive model. The simulation based ANN model was then run with the GA to optimise the process.

A third example is the use of a fuzzy logic approach based on GAs for plasma spray coating of zirconia.<sup>30</sup> Statistical design was first used to obtain sufficient experimental information to model the relationship between coating surface roughness and plasma spray process variables. Analysis of variance was then used to select the significant process parameters, which were then used to construct an adaptive fuzzy logic control model, using a fuzzy logic controller. A GA was then used to optimise the rule bases from the fuzzy logic controllers, based on the experimental data, producing a robust spray coating modelling tool. The final example is by Hsiang and Kuo<sup>31</sup> who produced an orthogonal array of the Taguchi method (experimental design) to define a good spread of input data of dies with different extrusion ratios (first determined by ANN modelling of

which die shapes gave which extrusion ratios) and combined this with other processing variables of magnesium alloys (including material type, other extrusion and die variables etc.) to assess the relationship between these processing variables and resultant tensile strength and extrusion load via ANNs, to allow optimisation of the extrusion process.

## Data mining

Industrial scale processing and manufacturing may potentially provide large, complex data sets from which improved process control, but also property prediction discoveries can be made, but the very nature of this data needs to be considered carefully. Although these datasets may seem an ideal exploitation area for a range of ANMs (due to their complex nature that is often not amenable to simple statistical inspection) the very nature of narrow process control often means that insufficient data space is explored to truly bring out materials science relationships. The datasets also often need considerable cleaning, filtering and checking to ensure that a sufficient quantity of high quality data is available for a meaningful modelling of what may be a high dimensional problem.

Talar<sup>32</sup> presents an evaluation of a range of data mining techniques for data analysis, modelling and control of metallurgical processes. The techniques presented include *k*-means clustering, decision trees, ANNs and Bayesian networks and a number of case studies are presented. Saxen *et al.*<sup>33</sup> describe some issues related to time series modelling of hot metal silicon content in a blast furnace, where approximation error and the number of weights for ANNs are minimised (optimised) simultaneously by a GA approach. Xiong *et al.*<sup>34</sup> examined the efficiency and capability of a recurrent neural network model used to predict damage evolution during hot non-uniform, non-isothermal forging on the basis of a limited number of snapshots during the process. A Bayesian algorithm was introduced to optimise the hyperparameters in the ANN related to the noise level (uncertainty in inputs and output predictions) and to the weight decay (the model fitting process). Owing to the lack of 'real world' (or experimental) data to fully interrogate the model, synthetic data (based on an existing relationship established between damage accumulation in a metal matrix composite as a function of strain, strain rate and deformation temperature) was generated of more widely varying accuracy and sparseness to assess the performance of the Bayesian algorithm.

Work at Southampton<sup>35</sup> has examined strength and toughness databases for a variety of commercially produced 2XXX and 7XXX alloys, which consisted of composition and thermomechanical data for individual production batches through the whole production process. Datasets contained up to 700 data lines with up to 14 input variables considered. A range of modelling techniques were compared: MLR, Bayesian MLPs, neurofuzzy models and a support vector machine derived approach with additional simple model representation based on the parsimonious ANOVA representation (SUPANOVA).<sup>9</sup> The key approach here was not only to consider a range of modelling approaches, but also to repeatedly sample and resample the train and test data splits (90%:10%) and examine the multiple

model runs for each technique, both in terms of averaged test MSE (effectively adopting a committee approach) but also in terms of underlying relationships revealed. The more complex ANM models outperformed the MLR approach, with the evaluation of predicted trends being considered a key element in assessing the model validity. The SUPANOVA approach was found to provide good modelling accuracy combined with global model transparency, unlike the Bayesian MLP which could only be interrogated over narrow cross-sections of the multidimensional input space via artificial datasets.

## Case study

While data sets from routine industrial processing may lead to a relatively narrow input space that will not support mechanistically broad model formulation, they may of course still have considerable value in process control and sensitivity analysis. Modelling of the commercial aerospace Al alloy plate rolling mentioned above by Christensen *et al.*<sup>35</sup> has for example been recently extended to explore the influence of alloy compositional variations on scatter in subsequent mechanical performance. This is particularly relevant as such materials are specified against conservative allowable values ('A values', 99% of the population exceeding the stated value with 95% confidence). In this case a committee of SUPANOVA models was interrogated with simulated input datasets (derived from real input dataset) representing hypothetical improvements in process control (*see* Fig. 4), where simulated process control in aluminium alloy plate production is shown: influence of reduced scatter in post-solutionising stretch (%St) on final strength distribution. While mean strength is essentially unchanged, the design allowable value is increased by ~7 MPa.

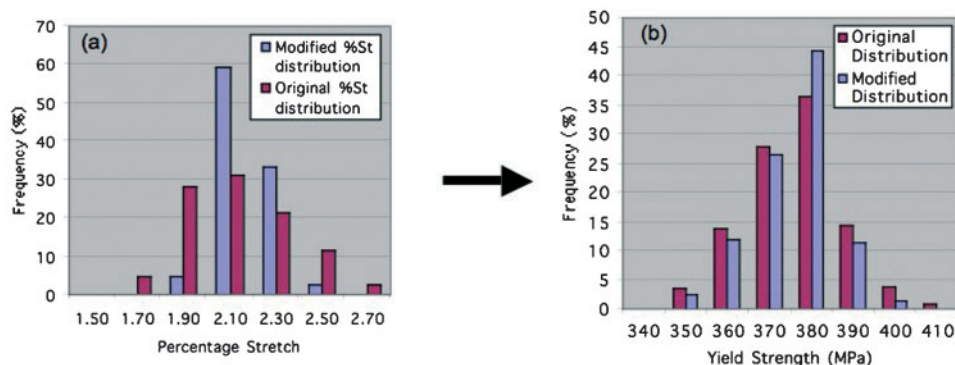
## Property predictions and interpolations of physically based models

### Physical and mechanical property predictions and thermodynamic predictions

A large number of papers have been written on property predictions using ANM approaches, most of which are regression rather than classification approaches. The properties modelled cover a wide range including: physical and mechanical properties as a function of manufacturing processes (e.g. welding) or alloy composition, thermodynamic predictions and fatigue initiation behaviour.

#### Physical and mechanical properties

Yoo *et al.*<sup>36</sup> used a Bayesian neural network to obtain a model for the creep rupture lives of single crystal Ni based superalloys as a function of alloy composition, creep stress and creep temperature, using a database which included literature data and original data from Rolls Royce. A Markov chain Monte Carlo method was required to obtain the posterior distribution in the Bayesian framework (and hence the confidence limit of the prediction). They specify a very particular architecture of their MLP and do not appear to have compared their model prediction with any other approaches, or to have assessed test/train data splits systematically, although they did assess model trends indirectly via examination of the automatic relevance determination



**4 Simulated process control in aluminium alloy plate production: influence of a reduced scatter in post-solutionising stretch (%St), on b final strength distribution. While mean strength is essentially unchanged, design allowable value is increased by ~7 MPa**

values provided by the model, which indicated Re and Cr had a significant effect on the creep rupture life.

Another rather simplistic example is given by Su *et al.*,<sup>37</sup> who constructed an optimal model of the aging processes of a Cu–Cr–Zr–Mg alloy using a supervised ANN to model the effect of aging parameters on hardness and conductivity, and then a GA to optimise the input parameters for these two outputs. This approach has not however been compared with any other ANM approaches nor has any model trend analysis been considered. Okuyucu *et al.*<sup>38</sup> have also used an ANN model rather uncritically to correlate the input parameters of weld speed and tool rotation speed in friction stir welding of Al plates to the output properties of yield strength, tensile strength, elongation and hardness of the weld metal and HAZ respectively. The present work simply states that the calculated results were in good agreement with measured data. Another approach is reported by De *et al.*<sup>39</sup> who studied pulsed gas metal arc welding of extruded 7005 Al–Zn–Mg alloys and generated six separate ANNs to predict individual outputs of ultimate tensile strength, percentage elongation, impact toughness, weld bead width, weld reinforcement height and penetration of the final weld joint as a function of peak current, base current, pulse on time and pulse frequency. They used committees of models to assess the uncertainty of the prediction, the individual ANNs were stated to model all properties (except weld penetration) ‘fairly accurately’.

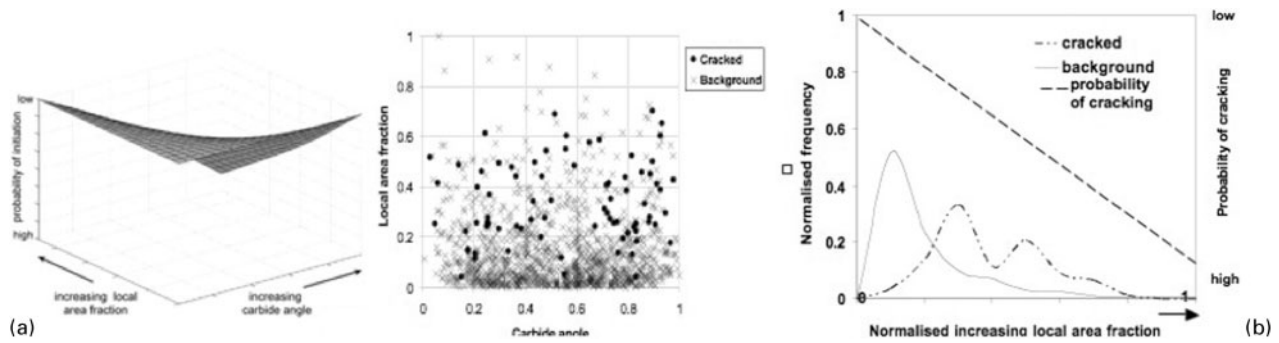
A more interesting approach is reported by Datta *et al.*<sup>40</sup> who have used two different methods to reduce network interconnectivity: a pruning algorithm and a multiobjective predator prey GA, which have been used for ANN modelling of the mechanical properties of steels, so as to reveal the relevant connections within the neural networks. Both approaches allow the least significant connections to be removed, this allows more knowledge to be extracted from the data, allowing the relative relevance of the composition and processing parameters to be revealed and to design a steel with a tailored property balance.

Keehan *et al.*<sup>41</sup> have used neural network models to identify possible alloy composition changes in high strength steel weld metals containing 7–9 wt-%Ni that would lead to improved fracture toughness or a balance of properties such as enhanced yield strength with limited reduction in toughness. Based on this they have defined a specific experimental test matrix to assess these

ANN predictions, which they have also compared with thermophysical or thermomechanical (using ThermoCalc software) model predictions and detailed microstructural evaluations to determine the microstructural features that may explain the ANN prediction. This is a good example of using the data driven ANN approach to define an interesting area of composition/processing space to explore and then moving on to assess on a more physical basis the reasons for optimised properties.

Kar *et al.*<sup>42</sup> used a Bayesian framework MLP to predict the yield and ultimate tensile strengths of Ti–6Al–4V at room temperature as a function of microstructural variations produced by a range of heat treatments. A range of stereological protocols were used to characterise and quantify microstructural features, although they only seem to use the MLP to link between observed microstructural features and tensile properties, rather than linking heat treatment to prediction of microstructural features and from microstructural features to predict mechanical properties which would be more amenable to comparison with metallurgical understanding. Two more modelling approaches are described in Ti alloys: Banerjee *et al.*<sup>43</sup> consider the development of two novel quaternary biocompatible beta Ti implant alloys. They have used a combinatorial approach to develop optimised compositions and microstructures by compositionally grading alloy samples using directed laser deposition, and then heat treating and hardness testing the layers to construct a database relating composition and microstructure to mechanical properties. These data have then been used to train and test fuzzy logic based ANNs, which have then been used to predict the influence of alloying additions on hardness and modulus (which has been checked by experiment). Malinov and Sha<sup>44</sup> have integrated a range of Ti alloy property models (based on MLPs trained and tested from literature data, for: time temperature transformation diagrams, processing property models, fatigue life and corrosion resistance models) to allow optimisation of the various inputs to achieve the desired combination of property outputs in a graphical user interface to allow ease of use.

In a rather different application area, Ozbulut *et al.*<sup>45</sup> studied the dynamic behaviour of CuAlBe shape memory alloy wires, by assessing the hysteretic behaviour of the wires using a fuzzy inferencing system, whereby input variables of strain, strain rate and temperature or prestress were used to predict stress.



a bivariate representation of carbide angle versus local area fraction; b univariate representation of local area fraction

**5 Typical SUPANOVA generated terms for classification of crack initiating carbides<sup>45</sup> with associated data spread**

Gaussian membership functions were used to fuzzify data for each of the input and output variables, and then values of the initially assigned membership functions were adjusted using a neural fuzzy procedure to more accurately predict the stress levels in the wires by comparison of test errors (on unseen data) of the predictions.

#### Case study

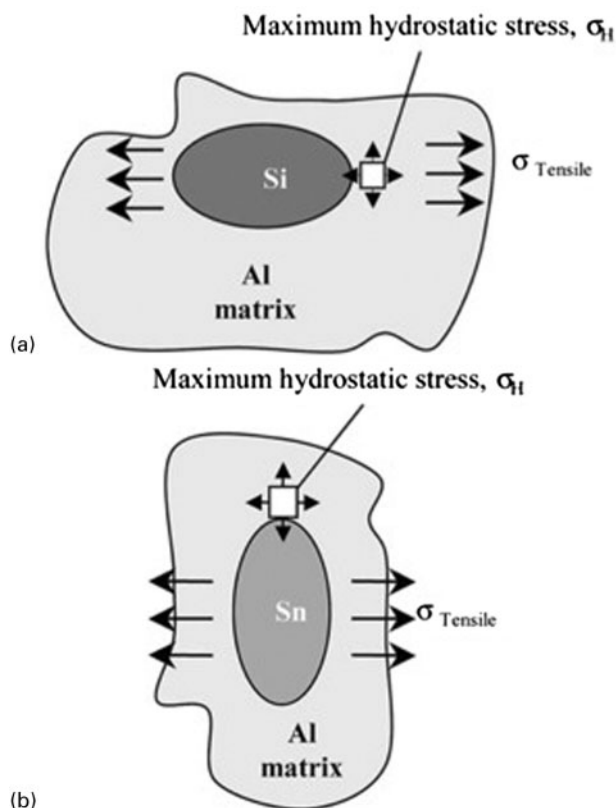
A number of papers from Southampton have now explored the role of secondary phase particle features (as derived from image analysis data) on fatigue initiation behaviour, which is an important process in components for which no reliable physically based models are available. This approach has been extended to assess the factors controlling fatigue initiation from low stiffness graphite nodules<sup>46</sup> or hard, brittle carbides<sup>47</sup> in austempered ductile irons, and to hard Si<sup>48</sup> and soft Sn<sup>49</sup> particles in a range of Al based plain journal lining materials. In each case a classification approach has been followed, whereby prediction as to whether a particular particle will fall into the fatigue initiation class or the non-initiation class is made as a function of finite body tessellation image analysis parameters that measure, size, shape clustering etc of the particles.<sup>50</sup> Unlike many classification techniques, which place an emphasis on obtaining a good classification rate (e.g. 100% successful classification of those particles associated with crack initiation), the SUPANOVA approach also provides enhanced model transparency and hence aids model interpretation (e.g. why do these particles cause initiation?). Such interpretation provides a valuable mechanistic insight and allows physically based optimisation of the process in question.

In applying the SUPANOVA classification, the initiating and non-initiating classes are defined. These two classes are typically a highly imbalanced data set (e.g. 90 samples for 'crack' and 1550 samples for 'non crack' in AS16, an Al based journal lining material),<sup>48</sup> the SUPANOVA classification avoids a bias operating for the more heavily represented class by use of differing misclassification costs and a Geometric mean  $G_{\text{mean}}$ , which favours a balanced classification by measuring the square root of the product of the class classification rates. A more detailed description of the approach taken to incorporate the differing misclassification costs and performance criteria for imbalanced data can be found in Lee *et al.*<sup>51</sup> The misclassification costs for each class are first tuned to obtain a good classification performance (based on  $G_{\text{mean}}$  of the unseen test data) using the pure SVM approach, using multiple partitioning of the

data into training and testing sets to provide multiple models. The SVM classification has no inherent transparency, and so the sparse ANOVA decomposition is next obtained for each model. The full ANOVA decomposition of the 11 possible tessellation features has 2048 possible terms ( $2^{11}$ ), but using the sparse representation approach adopted in SUPANOVA it was possible to reduce these terms without greatly compromising overall performance. Model inspection involved assessing which terms are most consistently picked out by the differing model runs on the different test/train data splits.

Figure 5 represents the relationships suggested by typical SUPANOVA generated terms for classification of crack initiating carbides<sup>46</sup> with associated data spread with a typical bivariate representation of carbide angle versus local area fraction and a univariate representation of local area fraction. The relationships predicted by the SUPANOVA classifier should be interpreted with caution, with particular attention being paid to the data spread and effective weighting, as shown in Fig. 5. Univariate relationships were often backed up by simple comparison of the relative population spacings of the two classes, giving increased confidence in the model trend selections, but bivariate or higher order relationships were typically too complex to be picked out by simple data inspection and revealed useful higher order interactions that informed our understanding of the physics of the problem. In the case of the hard stiff carbides in austempered ductile iron, SUPANOVA classification indicated that large or long and thin carbides that are locally clustered and aligned at a high angle to the tensile axis are particularly susceptible to fracture except when the nearest neighbour is perpendicularly aligned to the carbide with respect to the tensile axis. In the case of lower stiffness graphite nodules in austempered ductile iron, the critical crack initiating features were found to be a combination of nodule size and local clustering effects within a mesoscopic region containing a lower volume fraction of graphite nodules. In both these cases the important effects of local shielding were revealed in addition to well established load transfer effects.

In the case of the Al based plain journal bearings, inspection of the SUPANOVA classifier results indicated that the hard, stiff Si particles were more likely to initiate failure if they were larger and aligned with the tensile axis, whereas for the softer Sn particles the particles were more likely to initiate failure when perpendicular to the applied tensile axis. This can be



6 Particles aligned for preferential initiation, showing positions of maximum hydrostatic stress in *a* Al-12Sn-4Si and *b* Al-20Sn<sup>48</sup>

understood in terms of maximised hydrostatic stress around the particles, as shown schematically in Fig. 6, where the particles are aligned for preferential initiation, showing positions of maximum hydrostatic stress in Al-12Sn-4Si and Al-20Sn.<sup>48</sup> The SUPANOVA classifier has then been able not only to successfully classify which particles will initiate failure, but the transparency of the resultant models allows further mechanistic insight to be obtained. Such models can also be used in optimisation studies, where simulated particle distributions can be assessed statistically to identify fatigue resistant microstructures.

#### Predictions related to thermodynamic equilibrium

Another group of models in the literature deal with microstructure predictions that are dominated by thermodynamic equilibrium. Reddy *et al.*<sup>52</sup> used a MLP to estimate the beta approach curve and transus temperature for alpha/beta Ti alloys. Input parameters were alloy composition and heat treatment temperature, with the output being the beta volume phase fraction. Training and testing data was found in the literature and from new measurements. A sensitivity analysis was used to examine extrapolations of the model and to estimate the beta transus temperature for other Ti alloys. The authors claim that extrapolation was possible from their model unlike previous neural network models, in claiming this they seem to be showing that extrapolations beyond their input data set still gave predictions that were metallurgically consistent, which could be considered an inspection of their model in metallurgical terms that gave improved confidence. Guo *et al.*<sup>53</sup> have also used an ANN to model the beta transus

temperature as a function of alloy chemistry, which showed good agreement with test experimental data and with thermodynamic calculations. Two other papers modelled steel transformation temperatures, the bainite start temperature<sup>54</sup> and the martensitic start temperature<sup>55</sup> respectively using neural networks to model the effect of chemical composition (bainite) or chemical composition and prior austenite grain size (martensite) on the relevant transformation temperature, in these cases a more sophisticated (ANM) empirical modelling approach was being compared with either existing empirical linear regression models or thermodynamic predictions, allowing a degree of physical interpretation. The question arises what benefits these approaches may give over thermodynamic predictions or experimental measurements. Essentially these ANM approaches can be seen as flexible fitting functions allowing interpolation between hard won experimental or thermodynamic data.

#### Finite element or constitutive relationship interpolations

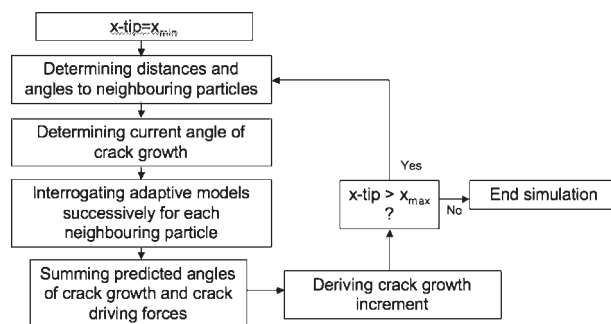
Another class of ANM reported in materials research is the use of these techniques for interpolations of constitutive relationships or finite element (FE) approaches, often with the aim of replacing the computationally expensive determination of constitutive relationships or FE approaches by the ANM model. Lucon and Donovan<sup>56</sup> used an ANN to calculate the global elastic properties of composite materials given the local microscopic properties and geometries (using an eight subcelled representative volume element) and found acceptable error values and greatly decreased computational time comparing with the traditional elastic micromechanical approach. Andrade-Campos *et al.*<sup>57</sup> examined a 16 parameter thermoelastic-viscoplastic constitutive model, where experimental data was obtained from tensile and shear tests at different temperatures for an AA1020-O Al alloy. The experimental data were used for comparison with the numerical results and also to determine (help fit) the correct material parameters in the constitutive model. Two different ANM approaches were used to determine/optimize these material parameters (i.e the fitting parameters in the constitutive model) a gradient based method and a continuous evolutionary algorithm method. The first method is very dependent on the starting point taken for the initial materials parameters and can end up optimizing in a local minima of the fitting function, giving very inconsistent results. The second approach is considered able to identify the global minimum in the fitting function much better. When the two techniques were compared, it was found that although the evolutionary algorithm method achieved a slightly better result it was computationally more expensive.

In some cases FE models can form part of the model chain required, or can be thought of as preprocessing input data for the ANM approach to allow property or microstructure predictions. Fratini and Buffa<sup>58</sup> examined the dynamic recrystallisation phenomena occurring in friction stir welding processes in 6082 Al-Si-Mg alloys, where they used as inputs the FE predictions of local strain, strain rate and temperature to predict the average grain size. This is similar to the approach taken

in an earlier paper<sup>22</sup> detailed in section on ‘Microstructure prediction models (including classification approaches)’. A related approach is reported by Li *et al.*<sup>59</sup> who studied the effect of hot deformation parameters on the microstructure of a Ti alloy by conducting isothermal compression tests and subsequent quantitative metallographic analysis. They then used ANNs to predict equivalent grain and recrystallisation volume fraction as a function of the hot isothermal compression parameters, which was then combined with a thermal mechanical coupled rigid viscoplastic FE model of hot extrusion and solution treatment to provide a combined FE ANN numerical simulation system of microstructure evolution/distribution for the process. Das *et al.*<sup>60</sup> have taken another approach where cellular automata hold microstructural features such as subgrain size and dislocation density, which are modelled by a neurofuzzy system that predicts the flow stress, these are embedded in an FE solver that can deal with the large deformations in metal processing. The method has been validated in a two-dimensional plane strain compression FE simulation for an Al–1 wt-%Mg alloy, where the model is shown to have the potential to incorporate the effects of underlying microstructure on the evolving flow stress fields, so highlighting the importance of understanding the local transition rules which affect global deformation.

Tyulyukoskiy and Huber<sup>61</sup> considered the problem of predicting mechanical behaviour from spherical indentation when such tips often deviate from the perfectly spherical, making the application of developed analysis methods uncertain. They used FE simulations for perfect and imperfect spherical tips indenting with varying material behaviour, as training data for ANNs which then solved the inverse problem of mapping the true tip shape and measured force depth curve to one that corresponds to the prediction for a perfect spherical indenter. Experimental verification was carried out for different spherical tips on nanocrystalline Ni and a Cu film on a Ti substrate. Liu *et al.*<sup>62</sup> had earlier tried a similar approach, using FE modelling of the load displacement due to a pyramidal microhardness indentation process, verified against experimental indentation data for materials with known elastoplastic properties. The FE simulations were then extended to an even wider range of materials variables to provide training data (inputs: load, elastic limit, yield strength, strain hardening coefficient and exponent; output: indent size) for a SUPANOVA ANM approach, where random 10%test–90%train data splits were used 10 times and the predictions averaged. The use of FE to expand and populate the available input space for the ANM model was considered particularly useful in view of limitations in available experimental data. The ANM was then much less computationally intensive to run than the FE simulation to identify elastoplastic properties for new materials.

Zhao *et al.*<sup>63</sup> have performed peel test measurements to estimate the interface toughness and separation strength between thin Cu films, with a range of thicknesses, and an Al<sub>2</sub>O<sub>3</sub> substrate. The interface parameters are deduced by an inverse analysis using ANN, where the interface parameters define the cohesive zone law in a cohesive zone model, and FE simulations based on strain gradient plasticity theory are



7 Flow diagram of crack path simulation approach used for Al–SiC failure

used to compare with the experimental data for one film thickness and thus deduce the interface parameters. The established interface parameters are then used in FE predictions for the other film thicknesses and are in agreement with the experimental results.

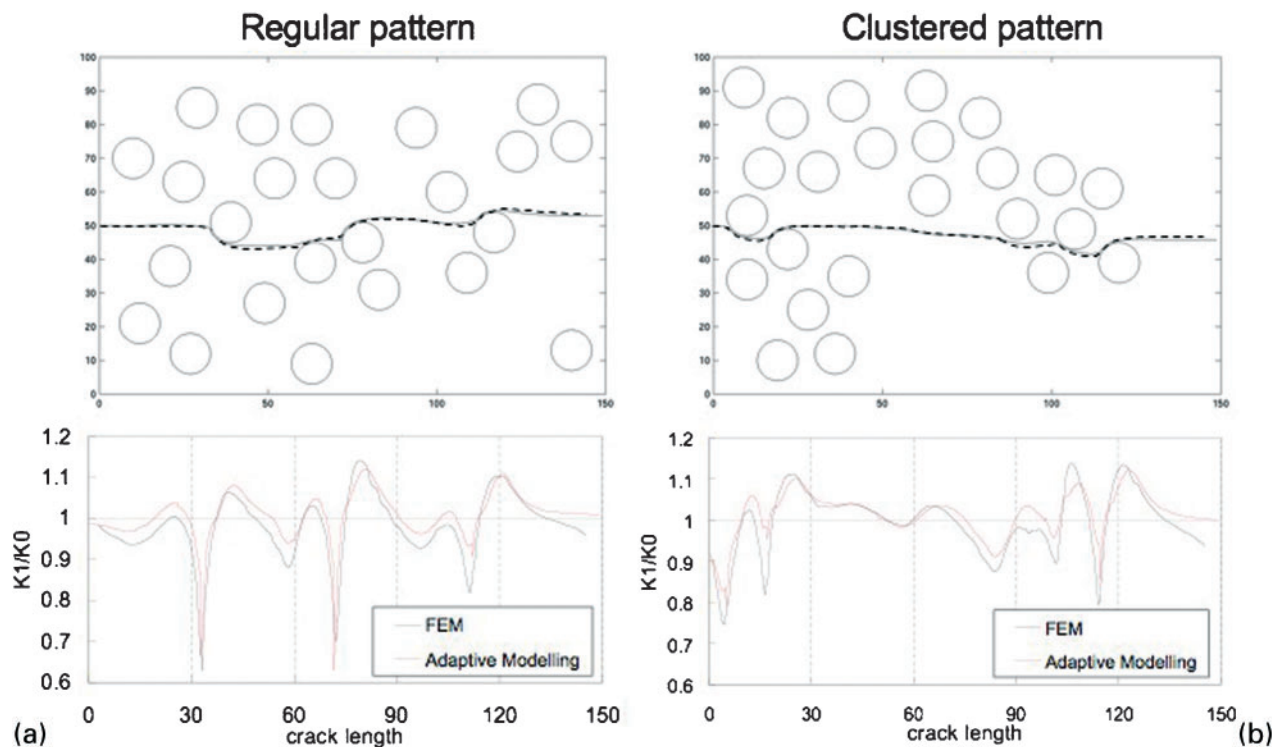
### Case study

This type of approach where computational efficiency of ANM interpolations can be seen to be particularly useful is some unpublished work by Boselli and Sinclair<sup>64</sup> who utilised a SVM derived response surface from a range of small finite element models of elastic–plastic interactions between a crack tip and reinforcement particles in a Al–SiC composite. Figure 7 shows the flow diagram of the crack path simulation approach used for Al–SiC failure. As such, crack growth across larger, more statistically significant sections of simulated microstructure could then be assessed than was otherwise realistic via FE calculation, as shown in Fig. 8.

These examples all show that ANM approaches are starting to take their place as one of the suite of modelling tools the authors can use in complex materials modelling problems, often as a useful interpolation device for materials data set representation.

## Hybrid ANM/physical modelling approaches

ANM integration in materials modelling can also be defined as hybrid ANM/physical modelling approaches. The framework of hybrid AN – physically based model approaches (APMs) has evolved in the interaction between AN modelling and physically based modelling. Its development inspired by the realisation that neither of the two techniques can on their own adequately deal with modelling problems in which physical knowledge is incomplete and available data is limited. This combination of circumstances is common in materials engineering problems. Deriving a hybrid APM starts by identifying mathematical functions that describe the relationship between (some of the) process input parameters (e.g. temperatures, time, compositions, exposure) and a key microstructure parameter that is dominating the property being modelled. Subsequently, these functions are used within a model optimising process to derive the full relation between input parameters and the property to be modelled. Thus hybrid APM aims to combine advanced numerical methods (and the ever increasing computing power available for it) with available physical understanding. As mentioned previously all applications of ANM to real world physical



8 Validation of SVM derived crack path (derived from local FE models) and full FE simulation for failure in Al-SiC composites for *a* random microstructure and *b* clustered microstructure, highlighting crack paths in relation to SiC particles, along with local fluctuations in stress intensity factor,  $K1$  (normalised against homogeneous material stress intensities,  $K0$ )

modelling issues involve some level of understanding of the physics of the problem; at the lowest level physical understanding is needed to define which input parameters need to be gathered. Hence it is not always obvious where the border between ANM and a hybrid APM lies. The authors will here provide some case studies of these approaches which fall well within the field of hybrid APM.

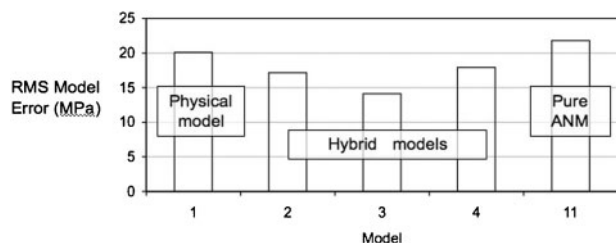
One of the earliest papers from Southampton<sup>65</sup> that used the inspection of trend prediction against metallurgical knowledge to choose appropriate adaptive numerical models compared two ANM techniques on the prediction of fatigue thresholds in Ni based alloys as a function of composition and test conditions. A Bayesian ANN and a neurofuzzy network were compared, both of which can automatically adjust the network's complexity to the training data set, although the neurofuzzy network is argued to offer benefits over the ANN in that it can restrict the complexity of relationships to the paucity of available data, and also provides transparent global output trend information (in the form of fuzzy rules) that can be reviewed in the light of metallurgical understanding, whereas the ANN can only do this after extensive interrogation/examination using simulated data.

Another early example from Southampton<sup>66</sup> concerns the prediction of strength and electrical conductivity measurements from compositional and aging time variants in the 7XXX series alloys comparing both multiple linear regression and neurofuzzy modelling approaches. To investigate the possible hybrid model formulations, the use of two input datasets was investigated: one to reveal more explicit microstructural information (e.g. precipitate volume fractions) and one

based on more empirical findings (e.g. critical alloying element ratios) reported elsewhere in the literature. The neurofuzzy modelling offered a transparent empirically based data driven approach that was combined with preprocessing (feature extraction) of the data and initialising of the model structure based on physical understanding. An iterative modelling approach was therefore defined by which data driven empirical modelling can be first used to assess underlying data structures which are then validated against physically based understanding, which then inform subsequent initialised neurofuzzy models and input data transformations to provide both optimal subset and feature representation.

Brown and May<sup>67</sup> developed a first order kinetic model to describe the mechanisms of anion exchange, surface desorption and diffusion during growth of GaAs<sub>1-y</sub>Py-GaAs superlattices grown on (001) GaAs substrates by molecular beam epitaxy, where high resolution X-ray diffraction was used to determine phosphorus composition at the interfaces. A semi-empirical hybrid ANN was then used to estimate the parameters of the kinetic model. Thus the ANM approach here has been used to determine the fittable parameters in a physically based model.

Abbod *et al.*<sup>68</sup> again report on their semiphysical hybrid model which predicts material properties such as stress-strain, recrystallisation behaviour and internal states in Al alloys as a function of temperature, strain rate and strain. The basic structure of their model uses a hybrid structure of neurofuzzy models and constitutive equations (which can be considered as more 'physically' representative) and is then embedded into an FE model used to calculate flow stress in plane strain compression



**9 Comparison of physically based, ANM and hybrid modelling methods applied to 7XXX series alloy strength predictions (six elemental and processing variables, 21 alloy compositions). Model performance is compared in terms of root mean squared (RMS) error against identical unseen data points**

tests, the same authors also report on similar work elsewhere<sup>69</sup> where these models are also compared with empirical models and in yet another paper<sup>70</sup> where they have used GAs to optimise the parameters used in the constitutive equations (which are used in the hybrid models). In the last example they assess the new hybrid model performance in terms of generalisation capability, simplicity of the model and smoother and more metallurgically convincing response surfaces (which can be considered an assessment of the metallurgical trend information in assessing the fitness for purpose of ANM).

Datta and Banerjee<sup>71</sup> modelled strength of thermo-mechanically processed High strength low alloy steels as a function of chemical composition, initially using a self-organising map (Kohonen network) which on inspection was rather poor at predicting unseen (test) data and did not follow on from metallurgical principles, as a result a learning vector quantisation method was adopted to provide more supervision during the learning process, based on physical principles, which resulted in good convergence/better prediction capability. This is another example of the 'pure' ANM approach being assessed/checked against physical understanding, and then modified in the light of physical/metallurgical knowledge.

### Case study

As a case study example, Christensen *et al.*<sup>72</sup> have assessed basic hybrid modelling benefits in strength modelling of 7XXX aluminium alloys: specifically some 21 alloys in varying heat treatments, giving 71 datalines, mostly for overaged alloys. A reasonable strength range was addressed, corresponding to ~200 MPa. Physically based, 'pure' ANM and hybrid modelling were considered. The physically based model was derived following Starink and Wang's<sup>73</sup> approach, while the pure ANM used SVMs, applied to elemental compositions and basic aging parameters (time and temperature). Several variants of hybrid modelling were investigated, combining different combinations of microstructurally derived input transformations, e.g. regular solution modelling<sup>74</sup> of phases forming and temperature corrected time during heat treatment<sup>75</sup> (as well as elimination of composition parameters that the physically based model predicts to be negligible). A broad comparison of model performance is shown in Fig. 9 in terms of RMS errors in unseen data: in this case a clear improvement in model accuracy may be seen for the hybrid approach, where a reduction in complexity may be identified in the input transformation.

## Summary and conclusions

The use of ANM techniques is well established and improved understanding of these techniques means they can now be used in a number of materials science applications.

Key issues to consider in utilising ANM include the following aspects.

1. Input and output data spread must adequately cover the problem space (and there must be sufficient data to support appropriately complex function fits). Design of experiment approaches can be particularly helpful here, and prior data inspection, filtering, appropriate input transformations can particularly help in checking this before applying ANM. Models that produce confidence bands or reliability indices on their predictions can be very helpful in indicating the data distribution that has informed the model.
2. Ensure that there is an appropriate complexity fit of the model to available data. This requires good knowledge of how the software package is actually obtaining the fits (e.g. what automatic model selection, optimisation and comparison procedures may be being followed), and users should be aware of any local minima issues in the objective function.
3. Critically review adaptive numerical models against other approaches, these can include: simple data inspection, trend examination (e.g. via sensitivity analyses) or indeed global trend extraction via use of more transparent modelling approaches, comparison with a physically based model or differing regression approaches (e.g. from classical statistics).

Transparency in models can be obtained in a number of ways, by progressive pruning to identify key relationships, or parsimonious representations of fuller model structures, or via sensitivity studies (although these can rarely give a global trend across multidimensional input space due to the limitations of representation in 3D)

The most exciting work in the ANM field in materials is now using ANM as one of many tools in a suite of modelling techniques, where these types of models can fit into multiscale models and can sometimes be considered as particularly clever interpolations. For example where they can be used to interpolate between hard won experimental or thermodynamic data, or to link between computationally intensive FE and constitutive models, where well spaced examples can define the data space and the ANM approach is a 'sensible' interpolation saving on processing time.

Another important area is in hybrid APM modelling, this can range from, at the most basic level: careful data selection (what does materials science tell us will affect the phenomenon?) data preprocessing (feature extraction) to transform inputs (e.g. manufacturing controls) into data that will directly affect the phenomenon being modelled (e.g. temperature, time, volumes or types of microstructural phases) or functional transformations (e.g. taking logs to reflect a likely exponential process). At the other extreme from these rather simple examples are the use of ANM fitting approaches to optimise the remaining fitting parameters in a more physically derived model, and this also links to the idea that the main strength in ANM approaches now lies in their comfortable integration alongside many of the other

modelling techniques the authors now have at their disposal in the materials modelling field.

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