DARE
DESIGNING ALLOYS for RESOURCE EFFICIENCY
NEWS March 2017

Welcome to our first issue of the DARE newsletter for 2017. In this edition we give an insight into some of the work we are doing as part of the Research Theme relating to Magnesium Alloys, together with an update of other news from the latter part of 2016 and planned events for this year.

Magnesium Alloys less dependent on Rare Earth additions

This area of research within the DARE programme is led by our partners at Kings College London in collaboration with our industry partner Magnesium Elektron. The aim is to find new Mg alloys which are formable, ductile, non-textured and free of strategically sensitive elements such as rare earths.

We are studying the effects that different substitute elements have on the stacking fault energy (SFE) of Magnesium through atomistic simulation.

We think of the atomic scale theory or *atomistic simulation* in metallurgy as another kind of microscope. If we knew the forces that bound atoms together, and we had big enough computers and good enough algorithms, we could follow the movement of atoms within a metal at various temperatures as a response to external loading and stresses generated by crystal defects.

In the initial stages of our work around magnesium alloys, Research Associate Lefteri Andritsos and PhD student Guy Skinner of Kings College London, under the supervision of Professor Tony Paxton, have been looking at the material properties of Mg through atomistic simulation with the aim of developing a general model for hexagonal systems which could be adjustable and transferable for our industry partners.

Initially, to understand the SFE in Mg, Lefteri looked at the complex crystallography of this hexagonal metal and calculated “gamma surfaces” on a number of crystallographic planes (fig 1). To do this he first used a “modified embedded atom method” (MEAM), and corroborated the results using density functional theory (DFT). However, neither of these methods are really satisfactory, one being too simplistic and the other too complex and over engineered.

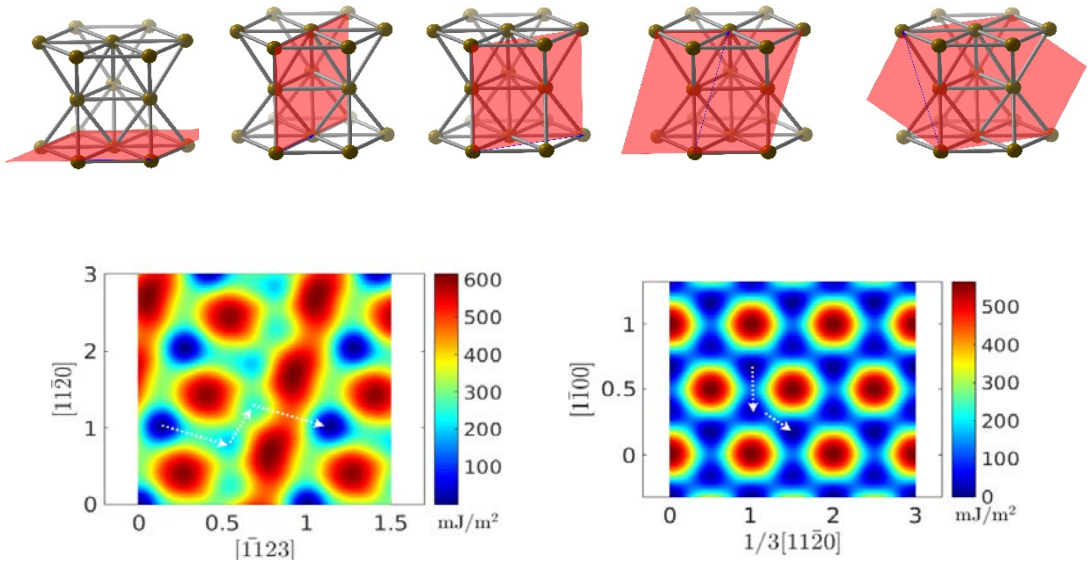

Figure 1: Gamma surfaces on pyramidal I and basal planes in Mg. These show a contour plot of the work needed to slide one half of the crystal over the other. The low contour paths dictate the structure of the dislocations.

What was really needed was a description of the metallic bond in Mg based on the first principles of quantum mechanics and which gave the research group a real insight into how to tackle the DARE alloy problem of large assemblies of metal atoms.

To carry out large scale atomistic simulations at constant temperature and stress it was decided to use the MGPT (model generalized pseudopotential theory) potentials developed by John A. Moriarty of Lawrence Livermore National Laboratory, California, together with a mathematical model developed by Guy Skinner. The latter enabled Lefteri & Guy to translate Moriarty's tabulated potential GPT energies into a smooth analytic pair potential acting between the multitudes of atoms in a specimen of metal. Through Guy's analytic treatment of the volume terms in the GPT functionals they were able to correctly predict the LO-TO splitting at the Γ point in the Brillouin zone; a very sensitive test which the MEAM fails. Lefteri also calculated the core structures of edge and screw dislocations using the GPT potential in pure Mg. The dislocation dissociation in both cases is in better agreement with results from DFT calculations than calculations with the MEAM potential. These are shown in figure 2 below.

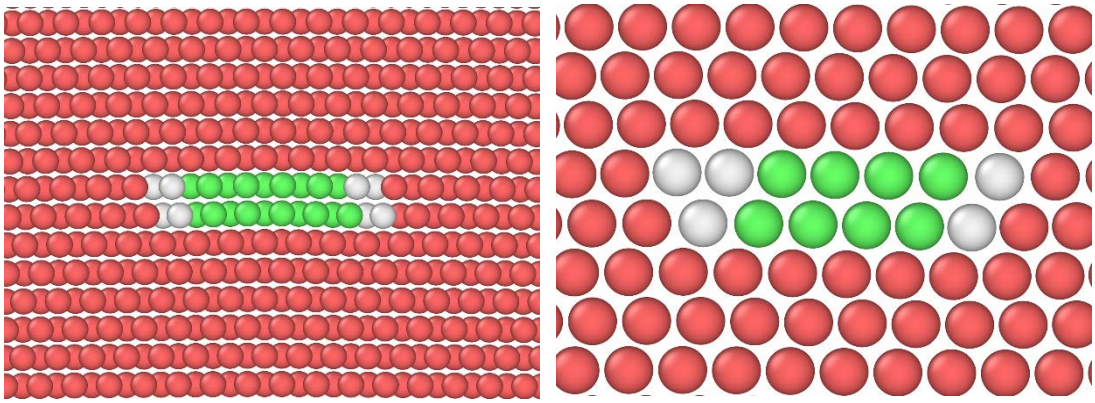

Figure 2: Core structures of the basal <a> dislocation in edge (left) and screw (right) orientations calculated using GPT. The splitting width into partials is consistent with DFT calculations and EAM except in the case of the edge which EAM predicts to have a width twice the DFT value. This shows the value of using quantum mechanics in deriving interatomic potentials.

We are now studying more complicated and relevant issues and currently considering calcium (Ca) as a substitute element in Mg. alloys. As part of this work we will be looking at:

- how Ca and other impurites alter the SFE and modify the structure of dislocations;
- how can we address the huge problem of plastic anisotropy;
- how is the Peierls stress affected by alloying;
- can we design cubic Mg alloys that will be ductile?

Our colleagues at Kings College are working closely with partners at the University of Sheffield and Imperial College, London to move this work forward; we will report on our findings in a later edition of our newsletter. For further information please contact:

Professor Tony Paxton Tony.Paxton@kcl.ac.uk **OR**

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Congratulations

New Fellows of the Royal Academy of Engineering 2016

Being elected as a Fellow of the Royal Academy of Engineering is one of the highest national honours that an engineer can achieve; amongst the list of names of new fellows elected in 2016 are **Professor Mark Rainforth, Director of DARE, University of Sheffield** and **Professor David Rugg, Rolls–Royce** (one of the Programme's industry partners).

Mark was recognised for his work in the use of advanced microscopy techniques that bring new insights into the understanding of friction and wear of materials. He has an outstanding worldwide reputation in this field. His research has led to new materials design concepts to enhance wear resistance that have now been adopted in commercial products.

David is distinguished for extraordinary contributions to the science, engineering and industrial uptake of hexagonal alloys at a world-beating level, and is a major element of the strength of the UK's titanium community. His seminal contributions include driving cold dwell and high cycle fatigue research and applying this to significant industrial issues.

DARE academic to lead one of the UK's new Future Manufacturing Hubs

Professor Iain Todd, an investigator in the DARE programme, will lead the new £10 million EPSRC funded "Manufacture using Advanced Powder Processes (MAPP) Hub". MAPP will focus on developing new powder-based manufacturing processes that provide low energy, low cost and low waste manufacturing routes and products for UK industry. Further information about the Hub can be found at the link below:

https://mapp.ac.uk

DARE Early Career researchers' achievements

Dr Enrique Galindo-Nava, University of Cambridge, has been awarded a Research Fellowship from the Royal Academy of Engineering. He will receive 5 years funding to advance his work in the development of novel materials for gas turbines using an integrated computational and modelling approach. Using modelling and experimentation Enrique's research will aim to optimise the properties of materials employed in gas turbine engines, whilst ensuring their appropriate manufacturability; this will build on the work he has been doing for the DARE programme in the design of new alloys and continue the theme of Resource Efficiency and Sustainability.

You can find out more about Enrique's work in the DARE programme and his future research plans at the following links:

http://darealloys.org/dare-annual-symp…ry-presentations/

http://www.msm.cam.ac.uk/department/profiles/galindo-nava.php

Dr Alexander (Sandy) Knowles, Imperial College, has been awarded a 2 year EUROfusion Researcher Grant Fellowship which will commence in October 2017. The EUROfusion Researcher Grants programme encourages excellence and career development of researchers who are already in the programme or high quality candidates from outside the programme. Sandy, who currently has an EPSRC doctoral prize fellowship, will continue to be based at Imperial College and his research will be linked with the Culham Centre for Fusion Energy (CCFE). He will be mentored by **Professor David Dye, Imperial College & PI of DARE** and **Dr Chris Hardie, CCFE**. For further information about his planned research please contact Sandy at the link below:

mailto:a.knowles@imperial.ac.uk

Dr Sam Tammas-Williams, **University of Sheffield**, was selected to present a poster at the recently held final of the **STEM for Britain** competition, Westminster. Sam, an early career researcher working in the Additive Layer Manufacturing research area of the DARE programme, presented and discussed his research to members of

both Houses of Parliament and EPSRC representatives after his abstract was chosen from over 500 entries in the competition.

Good luck to Mozart Queiroz Neto, who will attend the 2016 steel Challenge World Championships in Beijing, China during April after winning the European Regional Championships towards the end of 2016. Mozart is a PhD student at the University of Sheffield and some of his research is linked to the DARE theme "Advanced High Strength Steel". You can read more about Mozart and the competition at the following link:

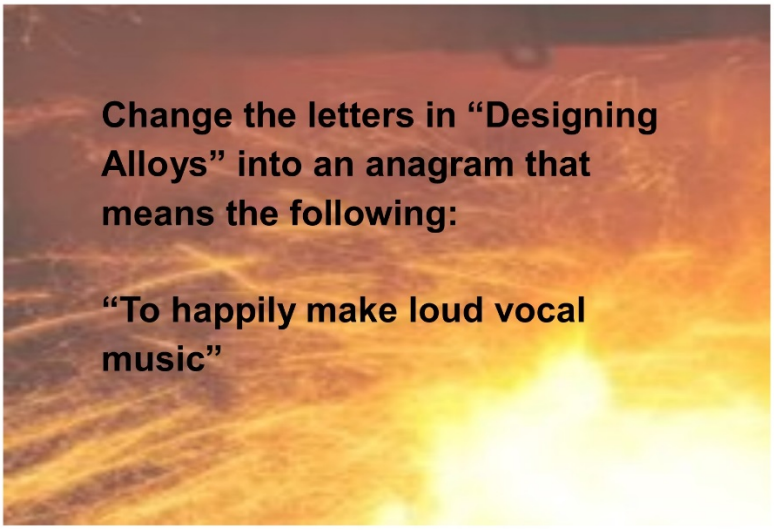
http://www.sheffield.ac.uk/materials/news/steelchallenge-1.667513

Events

Following our successful **Annual Symposium** in September last year, we have decided to hold this year's conference over two days. The Symposium will take place on **7th & 8th September 2017** at the **Rolls-Royce Learning & Development Centre, Derby** and will include a drinks reception in the Heritage Centre at the end of the first day. Further details about the programme will appear on our website in due course but you can win a free place to this event by entering the competition on the next page.

Competition

We are offering a free place at this year's Symposium to the first person to send the answer to the question below via the **form** on the **contact page** of our website.



For Further information about the DARE programme please visit our website http://www.darealloys.org or contact:

m.rainforth@sheffield.ac.uk ***or*** *jean.simpson@sheffield.ac.uk*