DATA-LED STRUCTURE ANALYSIS OF SIMPLE AND MULICOMPONENT CARBIDES AND PHASE NUCLEATION

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Background and Introduction: *In this work, as part of a main project in data led approach for developing advanced welding structures with complex carbides system, first principles calculation and python program based data analysis are combined to establish systematic data of carbides (MCx and M(C, N)$_x$) and multicomponent carbides (M_7C_3). A python program is used to develop systematic data and lattice misfit between of different compounds based on Atomic Simulation Environment (ASE) and crystallographic files of different format. The work shows that the combine approach is effective in developing deep data linking lattice characteristics to functional properties and material behaviours in manufacturing. The lattice misfit and energy analysis data could provide important data for establishing the effectiveness of potential compounds as a nucleation site for another phase of different melting points, which is more effective than individual data based empirical approach. The effect of different alloying elements (including rare earth (RE) elements) on the crystal structures of multicomponent carbides (M_7C_3) is studied. The combination of physical modelling data (bulk and interface) and engineering multiscale modelling offers an effective way in composition design and development for enhanced functional properties in carbide based welded hardfacings and other systems.*

Effect of Doping Elements (Cr, V, Mo, Ti, W, etc).; rare earth elements (RE) and defects on the structure and properties of multicomponent carbides

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Materials structure analysis and alloying data driven compound design considering structures and functional properties.

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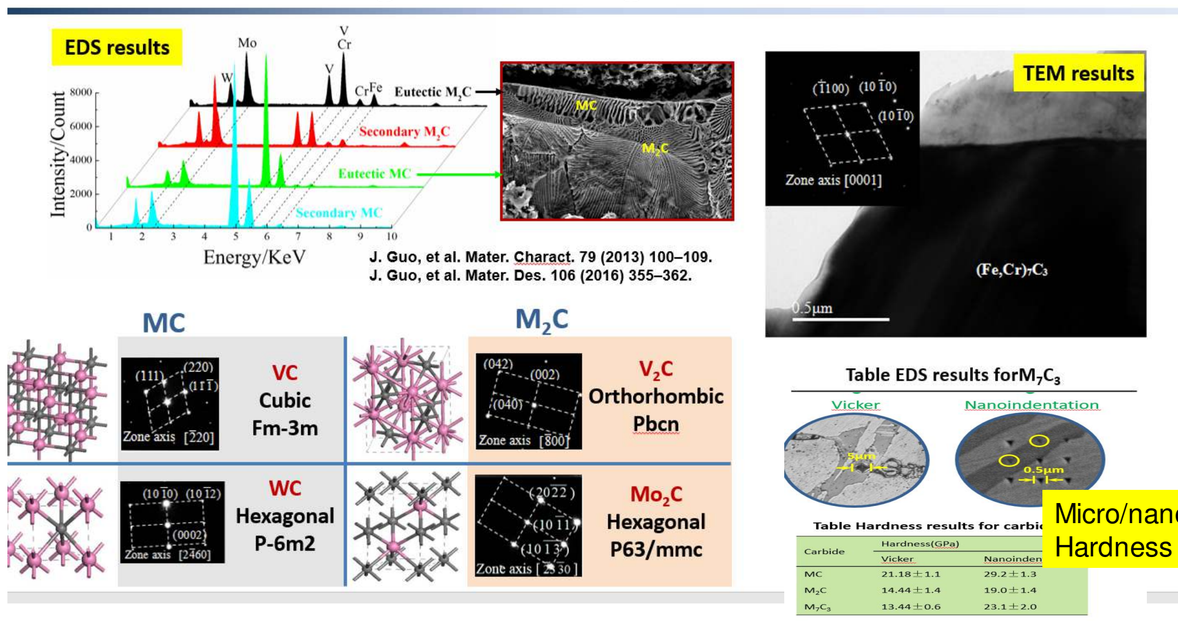
Effectiveness of different compounds as nucleation site for matrix and primary carbides for structure refinement and property enhancement.

Linking Physical Modelling and Engineering Simulation Through Systematic Data

Methods, Results and Discussion

Combination of testing and modelling



J. Guo, et al. Mater. Charact. 79 (2013) 100–109.
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Fig.1 Typical data showing the analysis and data for composition, crystal structures, characterisation and testing.

Fig. 1 shows that approach to study different carbide systems including simple carbides and multicomponent carbides. The bulk modulus, Young's modulus, shear modulus, and Poisson's ratio are determined from the Voigt-Reuss-Hill approximation method and compared with other published data. The micro Vickers hardness is also predicted and compared to published data. In the basic research part, over 30 carbides of different compositions relevant to compositions of welded hardfacings and other ferrous alloys were systematically analysed and the data established. The works on M_7C_3 has been focused on the effect of doping elements, such as Cr, V, Nb, Mo, W, Ti, etc, and rare earth (RE) elements. A typical example of (Fe, Cr)$_7$C$_3$ system is shown in Fig. 2. A range of doping elements has been studied, with the particular focus was on the effect of doping elements on the structure and lattice anisotropy. It is found that doping significant affects the a:c ratios of the M_7C_3 carbide systems which could direct affect the crystal nucleation/growth and the trade-off between strength/hardness and ductility.

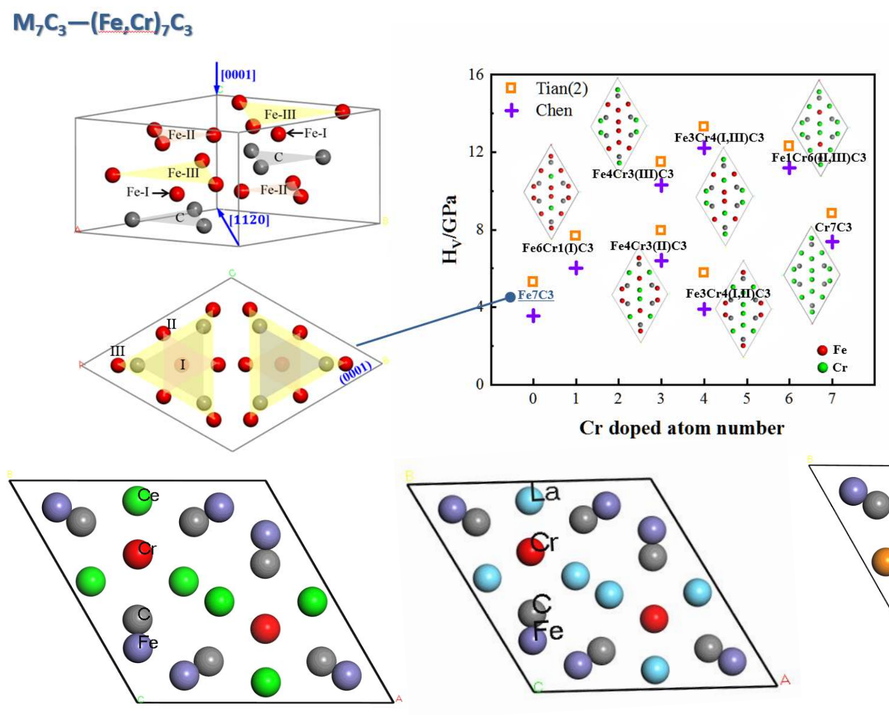

Fig. 2 Typical examples of structures with different alloying elements.

Fig. 3 Typical examples of M_7C_3 structures with RE elements (Ce, La and Y).

Nucleation is an important process controlling the microstructures of alloys and carbides. The effectiveness of a compound to act as a nucleation site is associated with the lattice misfit/mismatch values. A python program (Fig. 4) is developed to identify potentials of a simple carbides MC$_x$ and M(C,N)$_x$ as the nucleation site for matrix and other carbides. More complex compounds (e.g. Re-Al-O system) is also studied. Some example is shown in Fig. 5. The program is able to search different database of crystal structures with different format (e.g. Crystallographic Information File (.cif)) or using structure/group prediction/fitting systems (USPEX, CALYPSO, etc.). These data will provide a base for detailed interface studies to establish material model for engineering simulation through physical modelling.

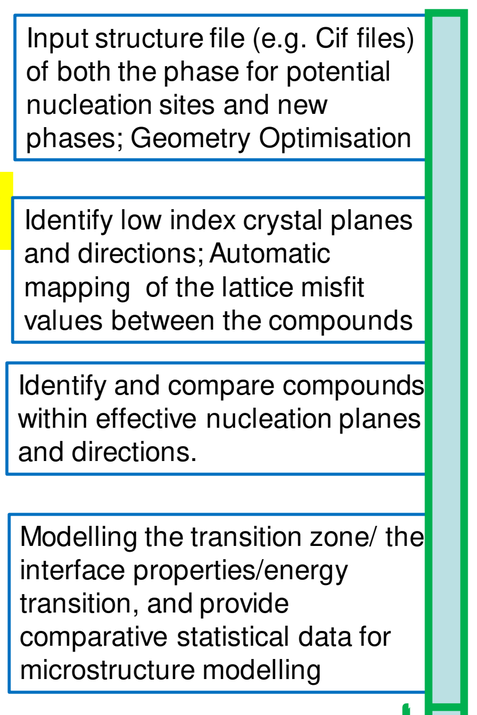

Fig. 4 Data structure and program for calculating lattice misfit between compounds and effectiveness of nucleation.

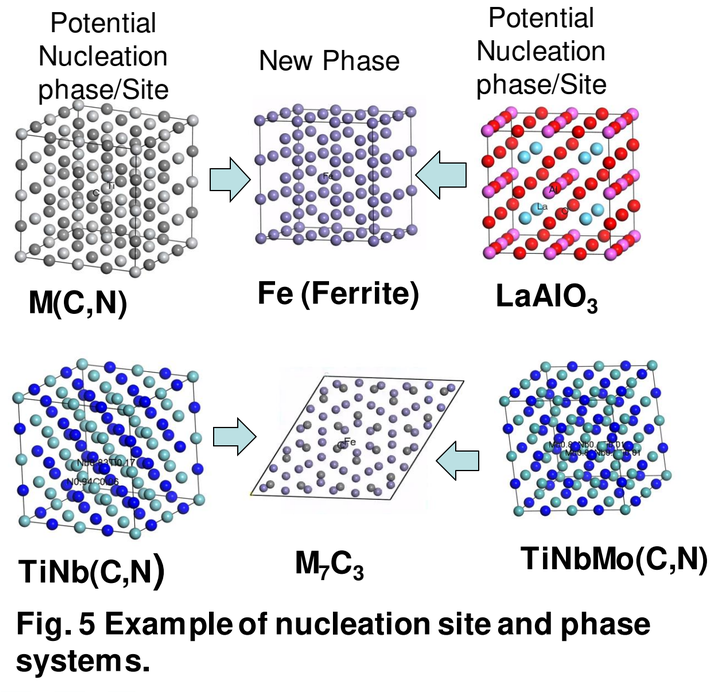

Fig. 5 Example of nucleation site and phase systems.

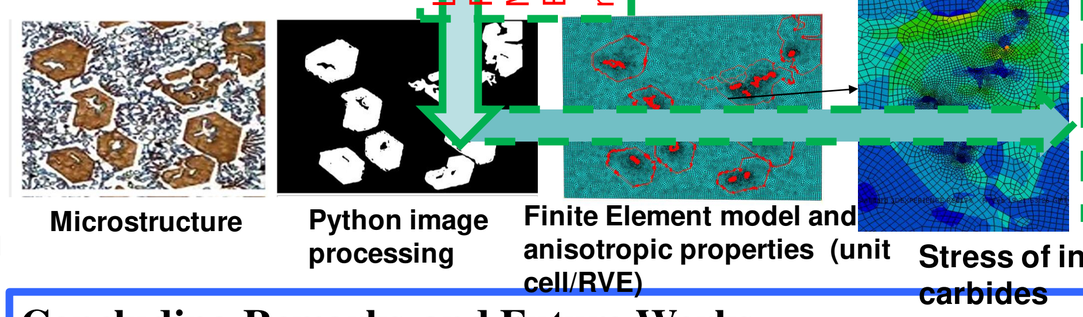

Fig. 6 Microstructure modelling of M_7C_3 carbides.

Concluding Remarks and Future Works

- The integrated approach and program is effective and efficient for dealing with complex material and processing issues, and the python program is a able to provide a systematic approach to map potential nucleation compounds/sites with statistically robust data.
- The doping elements showed different effects on the lattice parameters of MC$_x$/M(C,N)$_x$ and their effectiveness as nucleation sites for other low melting point phases. M(C.N) compounds are more effective and offers more composition design space.
- RE elements were found to be effective to tune the key characteristic (e.g. lattice parameter a:c ratio; anisotropy,) and improve both the hardness and the ductility.
- Linking physical modelling and engineering model is crucial for enhancing the use of physical modelling data for engineering applications. Interface is a key future challenge.

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