# Integrated Data-Led modelling of M7C3 carbides alloys

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**Background and Introduction:** *In this work, as part of a main project in develop data system for complex materials, different types of modelling including first principles calculation, python program, image analysis and FE modelling are combined to establish systematic data of carbides multicomponent carbides ($M_7C_3$). The work shows that the combine approach is effective in developing systematic data at different scales. The effect of different alloying elements (including rare earth (RE) elements) on the crystal structures of multicomponent carbides ($M_7C_3$) is studied. Feature analysis has been applied to a large quantity of carbides. A new approach is developed to model the structure of individual carbides including the stress concentration factors associated with the shapes and the internal features, which is critical to wear and fracture of the carbides. The combination of physical modelling and engineering modelling offers an effective way in developing integrated data for materials with complex composition and morphologies which is to be applied to different materials systems. .*

Effect of Doping Elements (Cr, V, Mo, Ti, W, etc).; rare earth elements (RE) on the structure and properties of multicomponent carbides ⇔ Effectiveness of different compounds as nucleation site for primary carbides. ⇔ Feature analysis and Microstructure Modelling: Individual carbides, Carbides aggregates, hardness, wear toughness

**Integrated Physical Modelling and Engineering Simulation for Systematic Data Development**

## Methods, Results and Discussion

### Combination of testing and modelling

$M_7C_3$—$(Fe,Cr)_7C_3$

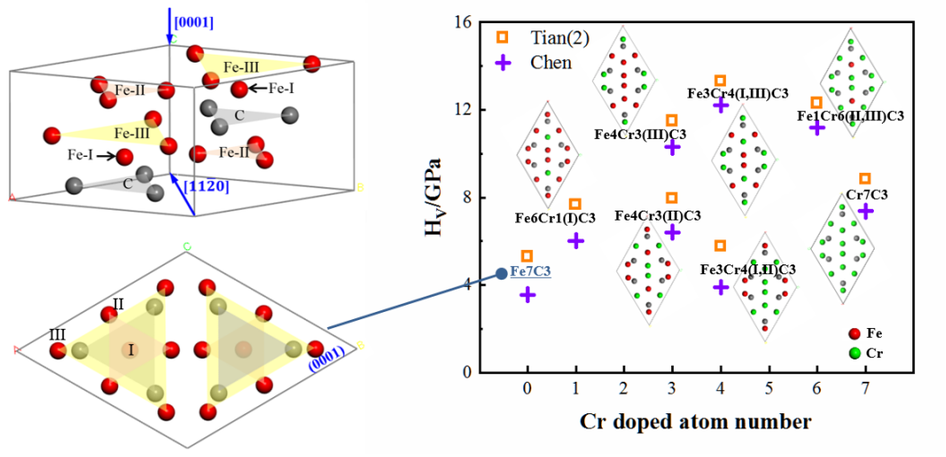


**Fig. 1 Typical examples of structures with different alloying**

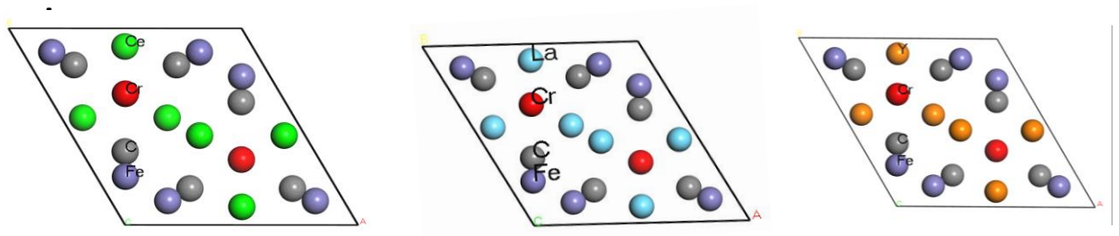


**Fig. 2 Typical examples of $M_7C_3$ structures with RE elements.**

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 $(Fe, Cr)_7C_3$ system is shown in Fig. 2. A range of doping elements have been studied, with the particular focus on the effect of doping elements on the structure and lattice anisotropy. It is found that doping significantly affects the a:c ratios of the $M_7C_3$ carbide systems, which could directly affect the crystal nucleation/growth and the trade-off between strength/hardness and ductility.

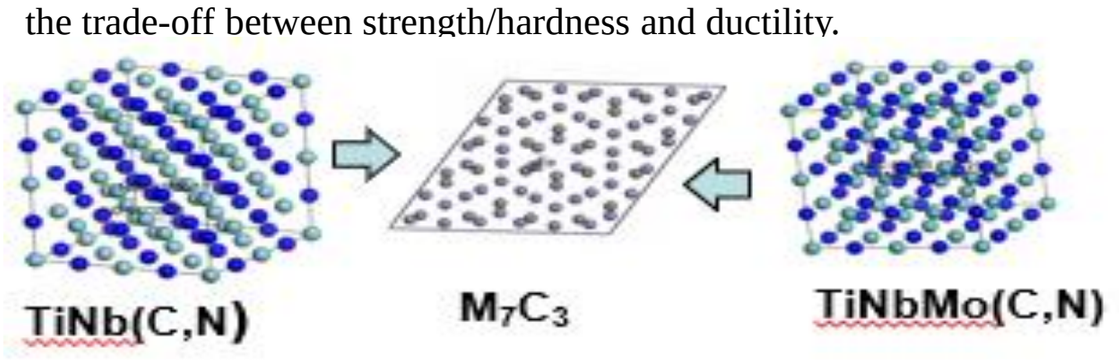


**Fig. 3 Typical combinations of simple carbides (nuclei) and $M_7C_3$ structures with RE elements (Ce, La and Y).**

Nucleation is an important process controlling the microstructures of alloys and carbides. Fig. 3. shows an example case of using modelling to evaluate the effectiveness of a compound to act as a nucleation site is associated with the lattice misfit/mismatch values. The work shows that both simple carbides $MC_x$ and $M(C,N)_x$ can act as the nucleation site for M7C3 carbides.

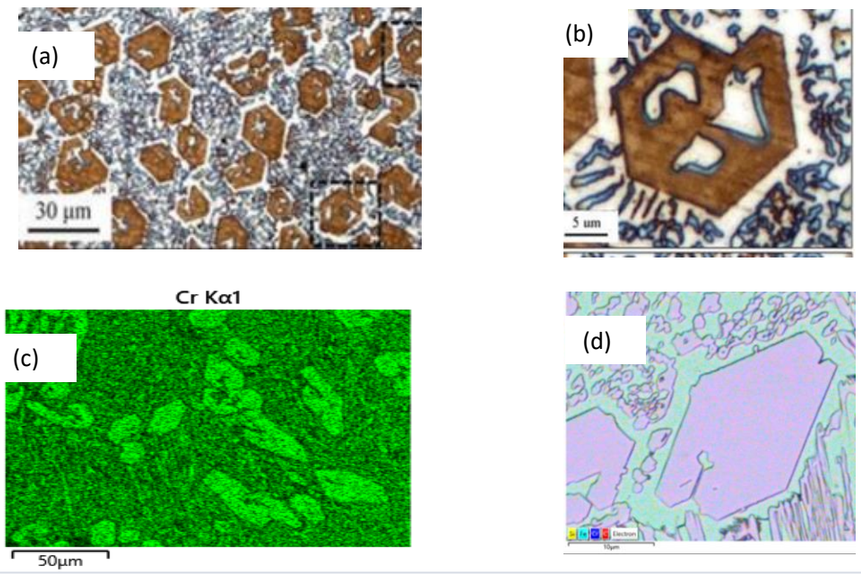


**Fig.4 shows typical Microstructures used in the feature analysis of M7C3 carbides for different sources**.
The work is focused on screening and classifying M7C3 carbides with different morphologies and develop a systematic data system of individual carbides (e.g. (b) and (c)) of different features (outline, internal regions, etc. )
As shown in Fig. 5, the program can predict the difference in overall deformation and the stress concentration, which is important for predictive modelling of fracture and deformation. The integrated data will provide an effective base for linking the structures of M7C3 to general properties as well as to other properties such as wear, machinability.

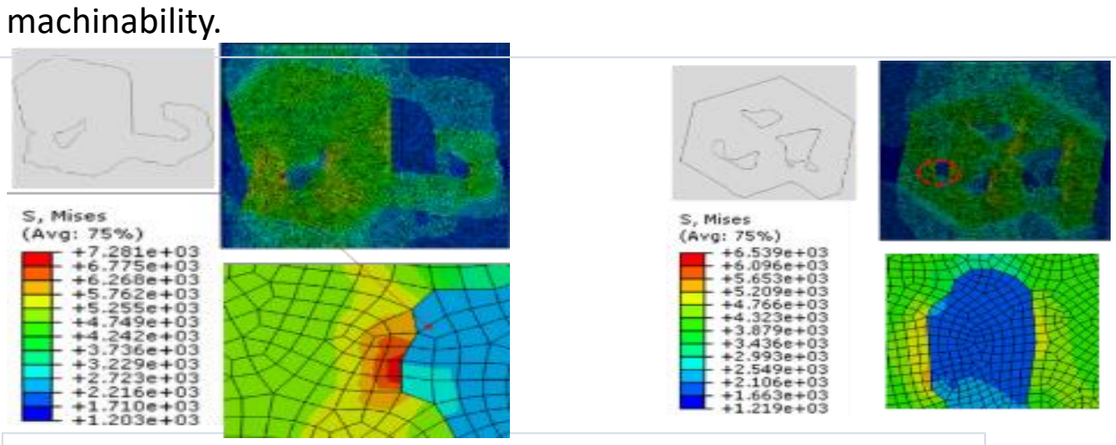


**Fig. 5 Typical microstructure Modelling of M7C3 carbide**

**Concluding Remarks: The integrated program is effective and efficient for dealing with material of complex shape and compositions. The doping elements showed different effects on the lattice parameters of $MC_x$/$M(C,N)_x$ and their effectiveness as nucleation sites for M7C3, which may have direct effect on the morphologies. Modelling of individual carbides are large scales will provide a more comprehensive information than simple homogenised data. Combining physical modelling and engineering model is effective in developing integrated data for material systems of complex compositions and shapes.**

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