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

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Abstract: The ground state structural and property data of different carbide systems (simple carbides (e.g. MC_x), multicomponent carbides (e.g. $(Fe,M)_7C_3$), where M represents different alloying elements (Ti, V, Nb, Cr, etc.)) are important for material development and processing. Carbides of complex compositions are widely used in key engineering ceramics and manufacturing tools as well as existing as secondary particles in various complex alloys. The structure and properties of secondary carbides directly affect the stiffness, strength, hardness, thermal conductivities and toughness of the alloys. The structural parameters of secondary phases also influence the nucleation and growth of metallic phases or other phases of different melting points (e.g. Ferrite, Austenite, M_7C_3, in steels and wear resistant welded hardfacings). Development of systematic structural data (e.g. lattice parameters, anisotropy) and the dependence of lattice characteristics on doping elements/defects in the crystals are important research areas supported by rapid development of computational tools. It will provide data for the predictive analysis on the effectiveness of secondary particle as nucleation sites for other metallic or ceramic phases.

In this work, as part of a main project, in developing data led approach in advanced welding structures of complex alloying systems, first principle calculation and python program based data analysis is combined to establish systematic data of simple carbides (MC_x and $M(C, N)_x$) and multicomponent carbides (M_7C_3). A python program is developed to analysis systematic data of functional structural characteristics and lattice misfit data between different crystals based on Atomic Simulation Environment (ASE) and Crystallographic Files of different format.

The work shows that the combine approach can effectively develop deep data linking lattice data to functional properties and material behaviours in manufacturing. Typical lattice misfit and energy analysis data reflecting the effectiveness of a compound as a nucleation site for another phase is presented and compared with data from previous works based on empirical approaches. The effect of different alloying elements (including rare earth (RE) elements) on the crystal structures of multicomponent carbides is studied. 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. The use of the physical modelling data in composition design and development for enhanced functional properties in carbide based welded hardfacings and other systems is discussed.

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