Data-led Analysis and Feature Based Modelling of Critical Phases in SS Welding & Joining

UNIVERSITI MALAYA

LIVERPOOL JOHN MOORES UNIVERSITY

IOCC 2024 Conference

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Background and Introduction: *Secondary precipitations and defects represent critical issues for joining advanced alloys in similar or dissimilar systems at different scales. Developing an integrated modelling and data system is essential for data-led materials design and processes optimisation. This work is concerned with developments of effective frameworks and data related to alloys associated with Fe-Cr-Ni system. The presented cases are focused on developing systematic data of secondary phases (inclusions and precipitations) in different systems including numerical models and molecule dynamics simulation. Typical experimental approaches for characterising more complex compounds (e.g. intermetallic and secondary phases with gradient depletion zones) is also highlighted. The in-process work demonstrate the importance of data at different scales for developing systematic knowledge for combined design of mechanical and functional properties.*

Typical cases and Data: Analysis of secondary particles

Data of precipitation is important for designing and managing the mechanical and functional properties (e.g. corrosion) and time -dependent behaviours (e.g. creep) of advanced materials. For different grade of stainless steels and welded joints, there are many different types of particles. A large-scale data collection has been conducted to establish the current trend and critical development areas. A typical example set of data is shown in Fig.1. The figure shows that main secondary particles related to duplex stainless steels in the past 10 years. Some main active areas included MnS inclusions (single phase or duplex phases). Work on nitrides is another active area.

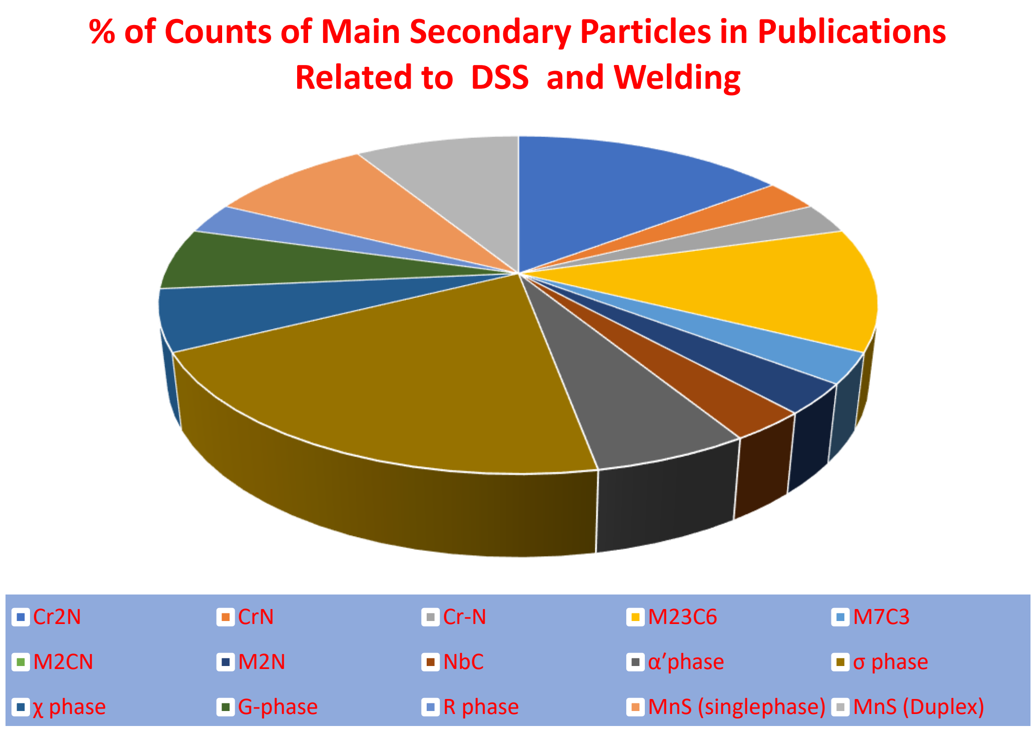

Fig. 1 Typical review data on secondary particles in DSS and related systems.

Typical Cases and Data: Modelling and Analysis of Inclusions

Fig. 2 shows some typical modelling work of MnS. One main focus of this model is the mechanical behaviours as many processes (such as fracture, debonding) will affect the corrosion process. A parametric template model is developed in Abaqus with functions of incorporating MnS with different morphologies. Multiple loads could be also considered including fracture of MnS under different loadings and temperatures. This will provide systematic tool and data to develop the link between shape/size of MnS on its effects in materials properties and behaviours. Such an approach can be extended to duplex MnS (such as MnS-Oxide and core and shell structures (MnS-Nb)), which are reported to be able to dramatically change the corrosion resistance.

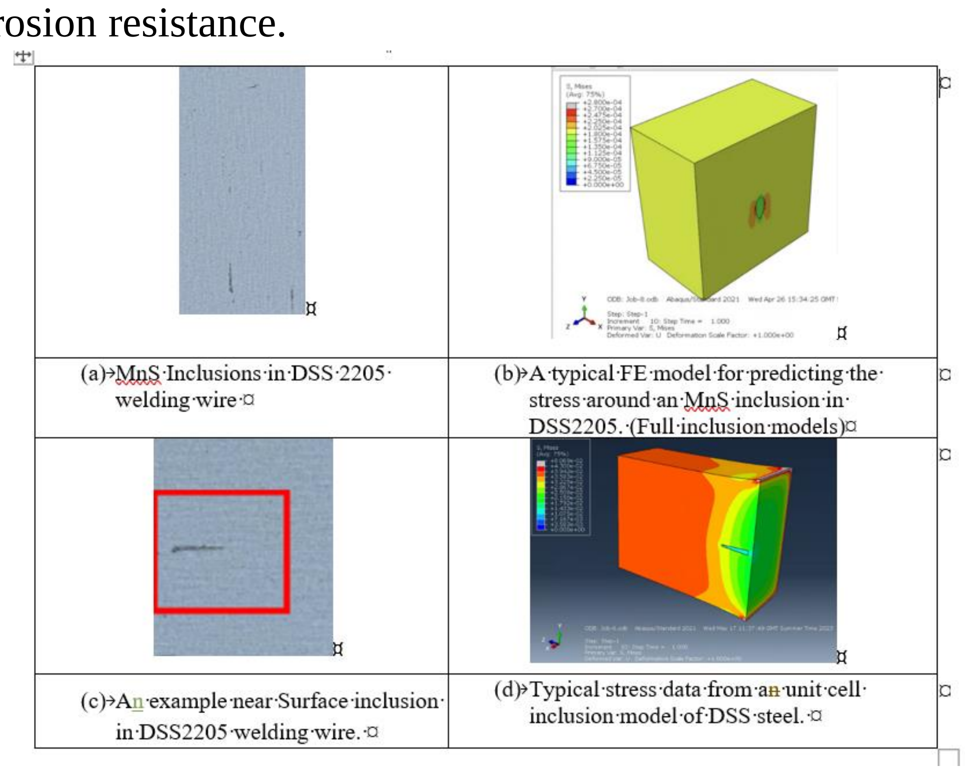

Fig. 2 Typical finite element models of MnS inclusions in DSS welding materials.

Typical cases and Data: Modelling and Analysis of Cr_2N

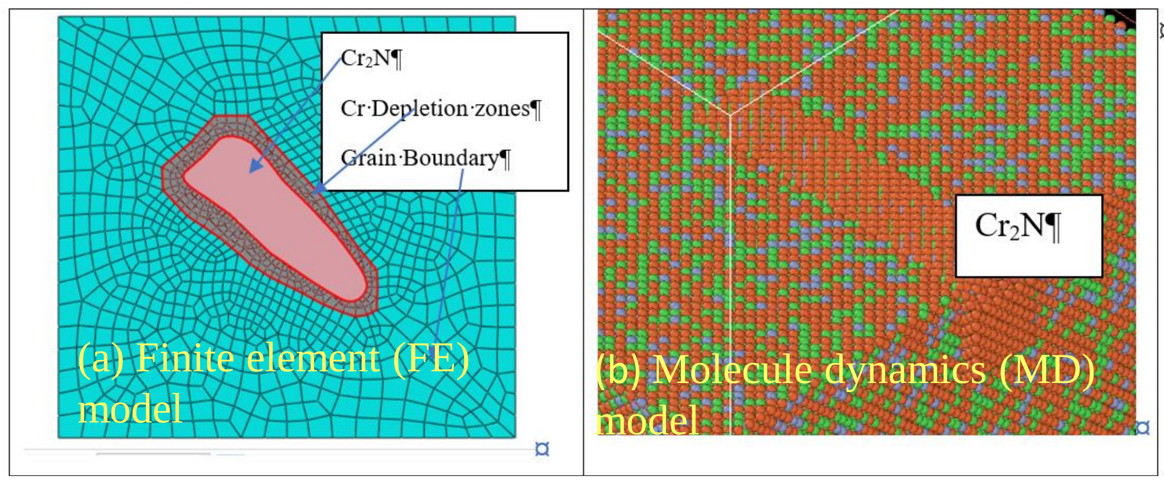

Fig. 3 Typical modeling approaches of Cr_2N and Cr-depleted zones.

Cr_2N is key precipitated phase in Fe-Cr-Ni system at the grain boundaries. Fig.3 shows typical Cr2N models at a grain boundary of duplex stainless steel. In the finite element model, the anisotropy and depletion zones can only be modelled through assigned properties. In the MD model (b), it is capable to incorporate the gradient change of composition directly reflecting the Cr depletion process. In addition, the integrated data will also provide more effective information to link the structure parameter (lattice coherence between Cr2N and the matrix) to complex mechanical behaviours (void initiation, etc.).

Typical cases and Data: Analysis of intermetallics (AlFe)

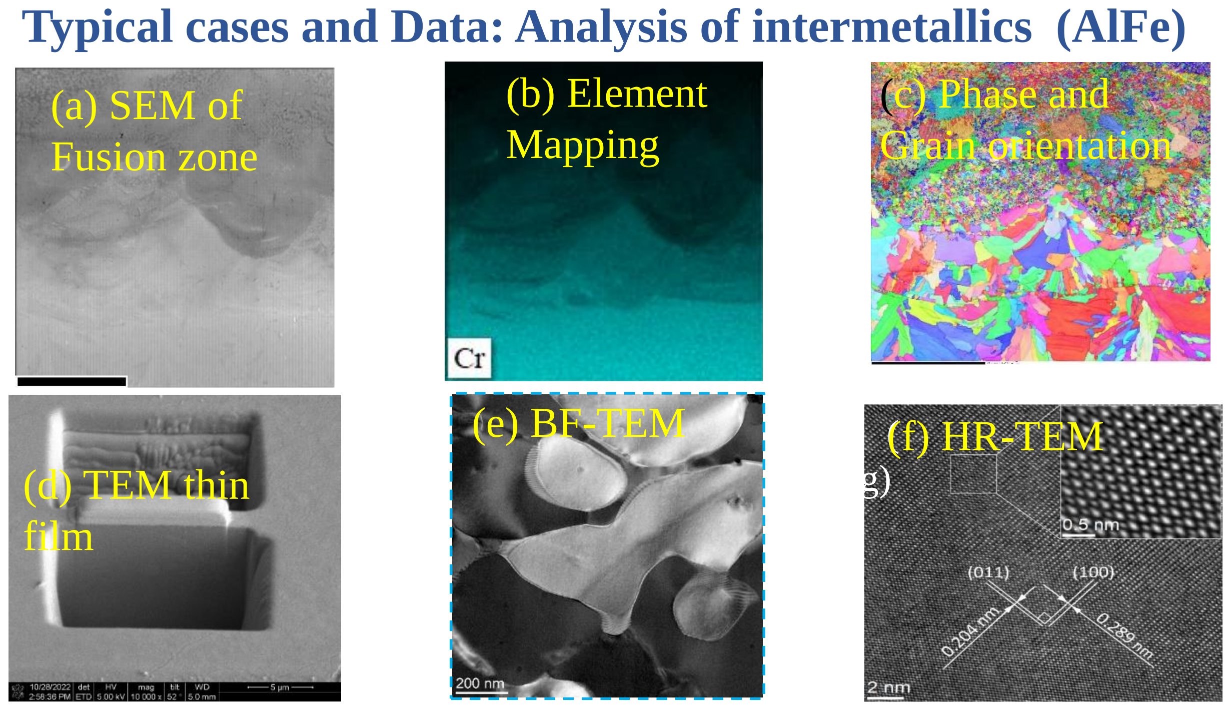

Fig. 4 Typical experimental data for characterising the structure and intermetallic in AlSi10Mg-FeCrNi joints.

Intermetallic compounds are difficult to model due to lack of data and large variety of compositions in different systems. Fig. 4 shows some typical experimental works employed to anlyse the fusion zones and intermetallic of a typical dissimilar system (AlSi10Mg and stainless steel). These experimental characterization is essential for FE and MD model development including development of interatomic energy function for new compositions. The TEM studies are important for establishing the lattice coherency data which is critical for fracture analysis and/or phase evolution under different conditions.

Concluding Remarks: The shared cases show that integrated modelling program is important for developing data for secondary particles in advanced stainless steel and joining in similar/dissimilar materials systems. Combining physical modelling and engineering model offers effective way in developing more information and knowledge which is important for data-led materials developments as well as education and training for workforce and AI program.

Acknowledgement: This project has received funding from Marie Skłodowska-Curie grant agreement No: 823786 and 101129996