Chapter 7

Conclusion

Within the framework of ab-initio DFT calculations, we investigated the effect of lattice parameter mismatch on the interface between the matrix of pure molybdenum, Mo and a carbide, MoC$_x$. This carbide is reported in an experimental study [64] as a metastable precipitate forming a semi-coherent interface at the grain boundary. This precipitate leads to the increase in the strength of the system by means of precipitation hardening. In the single crystal study carried out in our work, Mo and its carbides are investigated for the stable carbides using DFT. In our calculations, we observe the presence of metastable phase, MoC$_x$, that agrees well with the experiment. Mo with various carbon concentrations is analysed for the variation in formation energies and lattice parameters. Further, it is assumed in the experimental work [64] that the lattice parameters vary linearly with carbon concentration according to Vegard’s law by considering only two points, one at pure Mo and the other point at Mo$_2$C and interpolating linearly between them. In our work, we test Vegard’s law by considering the intermediate concentrations as well. It is found that the variation is non-linear with the carbon concentration. Vegard’s law assumes that the lattice parameter varies approximately linearly with concentration for the alloys with complete solubility in the solid state. In the case of our system, carbon does not dissolve but forms a precipitate. Hence the system does not follow Vegard’s law and this non-linearity is due to the transition from bcc to fcc structure via a bct structure.

The precipitation growth can be coherent, semi-coherent or incoherent with the original matrix of the metal. For modelling microstructure evolution or growth kinetics, the critical thickness of the precipitate is required. In our work, the coherent interface energy is calculated by considering the standard supercell approach with the interface between Mo and MoC$_x$. A previous computational study showed that there is a significant strain
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The interface model presented here allows for a variation of dislocation spacing as well as the dislocation core width. Taking these parameters into account and with coherent and semi-coherent interface energetics, we predict the critical thickness of the precipitate completely based on DFT results which describe the transition from a coherent to a semi-coherent interface. We predict a thickness of one to two atomic layers (lattice spacings) as the critical carbide thickness which agrees well with the experiment. The influence of temperature is considered analytically in the determination of the critical thickness in terms of thermal strain that in turn affects the mismatch in the system. It is found that the critical thickness increases with the temperature. With an increase in temperature, the size of the supercell changes resulting in different chemical energy across the interface from the one at 0K. Thus, this factor should also be considered in the calculation. As we have seen from the present work, the dislocation core width, the dislocation spacing and the
temperature affect the critical thickness of the precipitate. These factors must therefore be considered in the future. This model can be transferred to any other metal/precipitate interface in which a variation of crystal structure occurs across the interface with the phases being matched parallel to the interface. Further, the present DFT approach can describe any other interfaces as long as they can be represented by superlattices of moderate size. Then, misfit energies can be taken into account using results from the square lattice approximation obtained using the $\gamma$-surface results.