Interactions between Lattice Defects in Metallic Systems

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Summary

Several intermetallic compounds appear to have attractive properties for high temperature applications (1000°C). A typical example is given by Ni_3Al, which orders in a certain crystallographic structure (the $L1_2$ structure). This material shows a rise in its strength with increasing temperature (up to 800°C) and it is also chemically resistant. However, up to now one phenomenon has hampered the application of Ni_3Al: the occurrence of brittle fracture (fracture after very small deformation) along the grain boundaries (the interfaces between two crystals that have a misorientation with respect to each other). Normally, brittle fracture is attributed to de-cohesion of the grain boundaries.

This thesis demonstrates a different viewpoint. The research concentrates on the explanation of the occurrence of brittle fracture from both the crystallographic structure and from plasticity. Especially the interaction between dislocations (line defects that move under the influence of an applied stress) and grain boundaries has been studied. The degree to which the grain boundaries hinder the motion of the dislocations could be crucial for the occurrence of brittle fracture. Especially the effect of the ordering tendency has been investigated by comparison with other materials that have a lower ordering tendency and with mono-atomic materials that have a face centred cubic (fcc) structure. The fcc structure is topologically the same as the $L1_2$ structure.

The interaction between dislocations and grain boundaries has been investigated in an atomistic computer modelling study. In the simulations, a stress was applied to the lattice in such a way that a dislocation in the lattice would move towards the grain boundary. The simulations show that the interaction between dislocations and grain boundaries in $L1_2$ ordered materials is similar to the interaction in fcc, but that with a rising ordering tendency the grain boundaries form an obstacle of increasing strength against dislocation movement.

At first sight, one would think that grain boundaries have a specific structure for each misorientation and thus the interaction with dislocations would be specific for each misorientation. This study has shown that if the interaction mechanism is known for certain highly periodic grain boundaries, the interaction mechanism can be predicted for all the grain boundaries with similar misorientations. In this way, by studying only a limited number of grain boundaries, it is possible to draw conclusions that have a more general validity and applicability.

Next to the computer modelling studies, experiments have been performed in which Ni_3Al was deformed in-situ in a Transmission Electron Microscope. The interaction between dislocations and grain boundaries could be observed directly. The observations of a particular dislocation-grain boundary interaction could be compared with simulations of exactly the same system. Indeed, the interaction mechanism that was predicted by the simulations appeared to occur experimentally.

In conclusion, we can state that the interaction between dislocations and grain boundaries sheds a new light on the explanation of the occurrence of brittle fracture in alloys with high ordering tendency like Ni_3Al. Because of the hindrance of dislocation movement, stress concentrations will develop that will eventually lead to brittle fracture along the grain boundaries.

Samenvatting

Verscheidene intermetallis
bezitten voor toepassingen
motoren. Een treffend voorl
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Transmissie Elektronen M
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precies hetzelfde systeem
speld, bleek experimente

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