INTERDISCIPLINARY CENTRE FOR
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ICAMS special lecture

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What controls the choice of the slip system in different intermetallic compounds with B2 structure

The most common slip systems in B2 intermetallic compounds are < 111 > {101} and < 010 > {101} . However, different slip systems operate in different compounds and the question is what controls the choice of the dominant slip system. Answering this fundamental question is essential when investigating the ductility of B2 compounds since it depends primarily on operating slip systems. The dislocation property that is closely related and/or dictates the choice of slip planes and slip directions is possible dislocation splitting into partials, which depends on the existence of metastable stacking fault-like planar defects and their energies. Indeed, a common wisdom has been that it is the energy of the 1 2 < 111 > anti-phase boundary (APB) that is the decisive factor. However, unlike in FCC based structures, in the BCC based B2 structure possible metastable stacking fault-type defects are not ascertained by symmetry and thus the above mentioned APB may but need not exist. In fact, depending on the details of bonding and thus the electronic structure, the planar faults may be different in different B2 compounds or may even be absent. We investigated the existence of metastable stacking faulttype defects by calculating ! -surfaces for {101} planes in a number of B2 compounds (CuZn, NiAl, FeAl, PdAl, PtAl, CoTi, FeTi, NiTi and FeGa). These calculations were carried out using a density functional theory based method and, therefore, different electronic structures of different compounds were fully accounted for. These calculations reveal that in most cases the displacement vector of metastable stacking fault-like defects differs from 1 2 < 111 > while the fault with this vector is often unstable. Using the information about available metastable stacking faults and their energies we analysed possible dislocation dissociations in the compounds studied using the anisotropic elastic theory of dislocations. The conclusion of this study is that in order to decide which slip system dominates in a particular B2 compound three factors have to be considered: elastic anisotropy, displacement vectors of metastable stacking faults on {101) planes that vary from material to material and the energy of these faults. The analysis based on these three factors is in full agreement with experimental observations.