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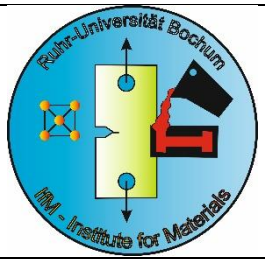

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Multiscale modelling of dislocation and plastic deformation in Magnesium and other HCP metals

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Mg, Ti, Zr and their alloys are technologically critical structural metals in lightweight, high strength or high resistance to corrosion applications. These metals all have hcp structure and exhibit strongly anisotropic, multiple slip behaviors, which are highly complicated and distinctly different among the hcp family and from those of well-established fcc and bcc metals. Despite their importance and continuous experimental and modeling efforts, our understanding on their atomistic deformation behavior is very limited. In this talk, I will present how a multiscale modeling approach, from density functional theory and empirical interatomic potential to molecular dynamics modelings and continuum theory, firmly establishes the fundamental dislocation, plasticity and fracture properties in Mg and other hcp metals. Density functional theory guided by crystal symmetry analysis is first used to obtain the fully-relaxed stacking fault energy, structure and fault vector on all relevant slip planes in a family of 6 hcp metals. The stacking fault information is then used as input to (1) elastic analysis to predict dislocation dissociation and relative dislocation energy, and (2) fit and validate an interatomic potential for simulating dislocation and fracture phenomena in Mg. The quantitative, elastic analysis provides a single framework able to capture the controlling energetics for different dissociations and slip systems across the family of hcp metals. Simulations based on the validated potential lead to a set of discoveries on unusual dislocation dissociation and cross-slip mechanisms. These new mechanisms are consistent with the elastic predictions, generic to all hcp metals, and essential in higher-scale modeling such as dislocation dynamics and crystal plasticity models. Furthermore, atomistic simulations and linear elastic fracture mechanics theory show that Mg is intrinsically brittle in many crack orientations and crack-tip geometries. The combined dislocation and crack-tip behaviors are the origins of low ductility and high hardening in Mg. The current multiscale approach not only reveals the rich, distinct, and complex behavior in the family of hcp metals, but also suggests fresh strategies to achieve high ductility in hcp metals, such as precise solid solution alloying to optimize cross-slip and enhance c-axis strain capacity, as well as to change crack-tip behavior for higher fracture toughness.

The *Materials Science and Technology Seminar* is jointly organized by *ICAMS* (Interdisciplinary Centre for Advanced Materials Simulation) and the *IfM* (Institute for Materials). Members of the *RUB Materials Research Department MRD* and of the *DGM Regionalforum Rhein-Ruhr* are cordially invited to participate in the seminar. For further information, please contact: Mrs. Christa Hermichen christa.hermichen@rub.de , phone: +49 234 32 29310.

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