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INTERFACIAL STRENGTH: AB-INITIO CALCULATION OF COHESIVE ZONE PARAMETERS

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ABSTRACT

It is a well established fact that the mechanical properties of polycrystalline materials, such as toughness and deformability, are determined to a large extent by the properties of their internal interfaces. Similarly, the reliability of coatings, multilayered structures and thin film devices strongly depends on the quality of and the adhesion at the heterophase interfaces. In all cases, the properties of the interface are determined by its geometry, the chemical composition, details of the atomistic structure, and the nature of the chemical bonds. Therefore ab-initio electronic structure methods are the method of choice for a computational study of these properties. They enable accurate and qantitative predictions of characteristic quantities, e.g. segregation energies, the work of separation, or energy barriers and critical stresses for grain boundary sliding and migration.

On the other hand, the actual dynamical process of deformation or delamination, based on grain boundary sliding, grain boundary migration, or crack propagation along an internal interface is determined by the microstructure on the mesoscale. Here, cohesive zone models have successfully been applied to model deformation, crack propagation and fracture of polycrystalline materials. In this approach the constitutive relations describing the mechanical behaviour of interfaces are given by so-called traction-separation laws. They relate normal and lateral forces to the normal separation and relative translation of the interfaces, respectively. The shape of these laws and the number of necessary parameters depend on the class of material.

In our studies we are bridging the scales between ab-initio and continuum methods. We determine the mechanical properties of interfaces with ab-initio methods, by calculating characteristic quantities and identifying the dominating processes of deformation for different kinds of interfaces. Based on this knowledge parametrizations e.g. for the works of separation or translation for different classes of materials can be gained and applied on the continuum level via cohesive zone models.

The first example, the adhesion of diamond or diamond-like carbon coatings on steel, illustrates some of these aspects. The adhesive layer system of chromized steel is split into individual model interfaces - the Cr/CrC_x and the CrC_x/diamond interface - which are investigated separately. From our calculated

values for lattice constants, bulk moduli, surface energies, and works of separation we can understand the principles that govern the adhesion at these interfaces. Interestingly, we find that stronger chemical bonds do not necessarily result in a stronger interface. As it turns out the lattice misfit plays the dominant role at these interfaces of crystalline phases. This is illustrated exemplarily for the Cr/CrC_x interface in figure 1.

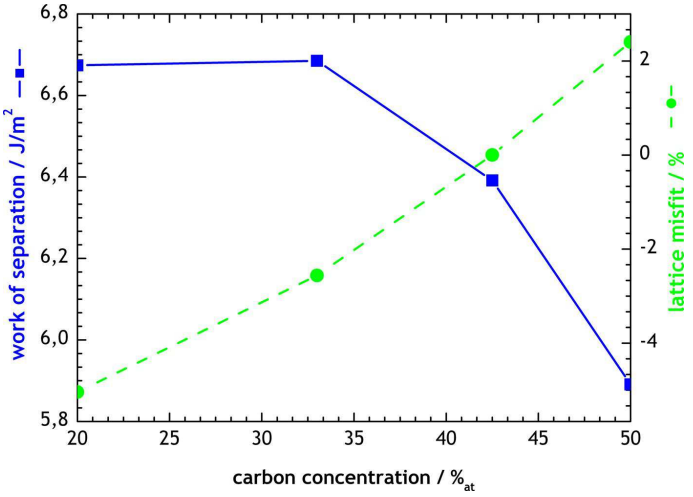

Figure 1: Work of separation and lattice misfit at a Cr/CrC_x interface for different C contents. With increasing C concentration, the lattice misfit between metal and carbide increases. The work of separation is lowered significantly in the compressive regime.

To develop a scheme to parametrize cohesive zone models with ab-initio results we choose a less complex example to start with, i.e. a series of special grain boundaries in aluminium. We calculate the works of separation and γ-surfaces for the grain boundaries with and without segregated impurities. Thus we can discuss the relationship between interface geometry, bonding character (and thus, to some extent the class of material) and the typical quantities for grain boundary sliding and decohesion. The extension to heterophase interphases as they occur in the coating system will be discussed, and the transfer to the cohesive zone model outlined.