New insights into ductility, defect energies and elastic stability in hexagonal close packed transition metals and alloys

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Abstract: Many hexagonal close packed (hcp) metals exhibit poor room temperature ductility and some display a ductile-to- brittle transition temperature: a well-defined temperature above which ductile behavior is displayed and below which brittle behavior occurs. Amongst refractory metals, hcp rhenium (Re) is uniquely distinguished by its absence of a measured ductile-to-brittle transition and its very high ductility. This makes the material particularly attractive for applications involving exposure to extreme variations in temperature. However, the usage of Re-rich alloys is inhibited by its high cost and worldwide scarcity. In this work, we employ first principles-calculations to study the fundamental physical underpinnings of the unique mechanical behavior of Re. First principles-calculations are used to assess elastic and defect properties of Re, from which intrinsic ductility parameters can be extracted. The high ductility of Re is shown to be related to its anomalously low twin boundary energy. We show that this twin energy anomaly is a general phenomenon occurring near a band filling of approximately 4.7-4.8 d-electrons per atom. It is further shown that this can be rationalized based on the local twin boundary structure, which is similar to the characteristic Frank Kasper icosahedral polyhedra that are observed in topologically close packed phases (TCP's). Our calculations show that twin boundary energies and elastic properties in hcp metals and alloys are strongly influenced by filling of the d-bands. This suggests avenues to create new alloys without Re, but exhibiting similar attractive behavior. In fact, recent calculations suggest new alloys which may serve as Re replacements, exploiting the twin energy anomaly near Re band filling. We finally show results of ideal strength-calculations, which provide further insight into ductility in hcp metals and which may be able to distinguish between ductile versus brittle failure. Some of our findings regarding Re-alloys are put in the perspective of recent efforts by the Materials Project to incorporate elastic and mechanical properties into the database.