Post-Doctoral Position on grain-boundary debonding in Al and H embrittlement using DFT calculations

This work is part of a multi-scale modeling project funded by Labex (Lab of Excellence) "Science and Engineering for Advanced Materials and devices" (SEAM). This project regroups a dozen of permanent researchers from three different laboratories from Univ. Paris 7 and Paris 13. Simulations ranging from the atomistic scale up to the component lengthscale are part of this project.

Context and job description

In polycrystalline materials, fracture is often initiated at weak spots of the microstructure, such as grain-boundaries, triple junctions or around precipitates. Crack initiation at grain boundaries is affected by several parameters such as temperature, plastic activity within grains, dislocation accumulations at grain boundaries, or the presence of impurities. Among these impurities, hydrogen atoms diffuse toward grain boundaries and reduce their cohesive energy (phenomenon known as Hydrogen Embrittlement). In consequence, the exact conditions, e.g. when and where debonding will start within a given microstructure, are still not precisely known.

The objective of this post-doctoral work is to improve our understanding of the hydrogen-assisted intergranular fracture by providing a complete cohesive formulation for a given number of grain boundaries of interest in Al. To this goal, DFT calculations will be employed since the strength of a grain boundary is intimately controlled by its atomic structure. The effect of local stress, temperature and H concentration at grain boundaries will be investigated. The set of grain-boundaries of interest will be provided by experimental observations conducted in parallel within the consortium.

The applicant will be recruited by Itodys (Univ. Paris 7) and will spend approximately half of his time at LSPM (Univ. Paris 13).

Applicant profile

A good candidate should hold a recent PhD degree in Materials Sciences, Mechanical Engineering, or Physics, with a strong expertise in Density Functional Theory calculations (VASP knowledge preferred) and their application to metals.

Applicants should join:

1) a resume including a list of publications and references,
2) an application letter,
3) a statement of research,
4) at least one recommendation letter.

The Application deadline is set to the 15th of February 2015.

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