Understanding grain boundary embrittlement and its correlation with polycrystalline tungsten fracture

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ABSTRACT

Grain boundary (GB) embrittlement has been repeatedly reported in fracture of refractory metals. It is suggested that the GB embrittlement is due to ductility loss by material addition and its segregation. Although there are a few hypotheses available, one of the guiding explanations is that mechanism of GB embrittlement by segregation is from creation of a barrier to dislocation propagation by formation of a hardened region near the boundary. In case of tungsten (W)–nickel (Ni) alloy, ductility loss by Ni addition is known to be not related to the change of grain size, however, geometry of GBs is found to have high dependence with the GB embrittlement as well as material properties of W. GBs in W-Ni alloy are found to have thickness as a function of the level of saturation of W atoms with respect to Ni atoms in the GBs. This study focuses on both atomic scale and continuum scale. The study in atomic scale examines (110)-(210) W GB mechanical strength as a function of thickness using an ab initio calculation framework based on Car-Parrinello molecular dynamics (CPMD) simulations. The atomic fraction of Ni atoms is varied to understand the influence of an addition and its correlation with thickness variation on the GB fracture strength. Based on the analyses performed, an analytical relation to predict GB peak tensile strength as a function of atomic cohesive energy, GB thickness (level of saturation), and the Ni atomic fraction is proposed. Then extended finite element method (XFEM) simulations have been conducted in continuum scale, with applying obtained GB peak tensile strength in atomic scale, to derive GB embrittlement in quantitative expression by introducing revised brittleness index, which takes account of length-scale effect.