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Multiscale modelling of gallium induced embrittlement in aluminium VENKATA SAI PAVAN KUMAR BHOGIREDDY, MIRA TODOROVA, Max Planck Inst für Eisenforschung GmbH, ROBERT SPATSCHEK, Research Center Jülich and Max Planck Inst für Eisenforschung GmbH, JÖRG NEUGEBAUER, Max Planck Inst für Eisenforschung GmbH — Liquid metal embrittlement is a degradation phenomenon in which a solid metal undergoes brittle failure when it is stressed while in contact with a liquid metal. The transition from ductile to brittle metal failure manifests itself by rapid crack propagations which reduces the elongation to failure ratio. Combining density functional theory calculations with continuum methods, we study the liquid metal embrittlement of aluminium in contact with gallium. Comparing ab initio calculated energies for a $\Sigma 3$ and a $\Sigma 5$ Al grain boundary and their corresponding surface energies in the presence and absence of Ga, we identify critical Ga concentrations which result in a weakening of the mechanical strength of aluminium. Parametrising the DFT results in continuum model we obtain the concentration as a function of the strain in the system. In a final step we extend this approach and compute the stress field induced by cracks in bulk and at grain boundaries. The stress field explains the large segregation of gallium atoms at the crack tip and the crack tips subsequent propagation.

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