

# Impurity-induced grain-boundary embrittlement: A simple three-dimensional model

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The impurity-induced grain-boundary decohesion is investigated on the basis of a three-dimensional-model calculation. The grain boundary is simulated by self-consistently modifying the hopping integrals between two neighboring grains and the impurities segregated there. We find that, for a wide range of parameter values, grain-boundary decohesion does occur. © 1990 The American Physical Society.