Incompatibility Stresses at Grain Boundaries in Strained Materials

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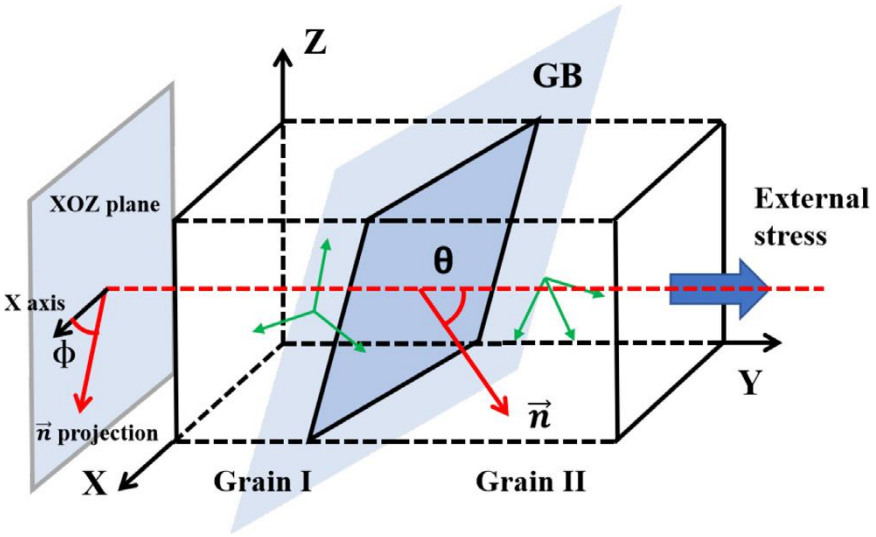
In a material under stress, grain boundaries may give rise to stress discontinuities. The stress state at grain boundaries strongly affects microscopic processes, such as diffusion and segregation, as well as failure initiation, such as fatigue, creep, and corrosion. The general condition of such incompatibility stress at grain boundaries is studied with a bicrystal model for linear elastic materials. In materials with cubic crystal structures, it is proven that hydrostatic stress does not contribute to a stress discontinuity at grain boundaries. For bicrystals with inclined grain boundaries under uniaxial stress, the extreme values of the incompatibility stress as a function of the inclination angle are obtained by a simulated annealing method. A simple criterion is proposed to classify cubic materials into three groups. For cubic crystals with at most moderate anisotropy, the highest incompatibility stress occurs when the grain boundary plane is perpendicular to the uniaxial stress. For highly anisotropic materials, such as alkali metals and polymorphic high-temperature phases, the highest incompatibility stress occurs on grain boundaries with an inclination of about 47°.



Schematic figure of the bicrystal model with inclined grain boundary under uniaxial external stress. The orientation of the grain boundary is defined with θ, the angle between the grain boundary normal $\vec{n}$ and the global Y-axis, and ϕ, the angle between the projection of $\vec{n}$ on the XOZ plane and X-axis.

References

1. Liu, K.; Sluiter, M.H.F. *Scripta Materialia*, **2023**, 234, 115570:5.
2. Liu, K.; Sluiter, M.H.F. *Materialia*, **2024**, 34, 102071:8.