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# Molecular Dynamics Study on the Strain Rate-Dependent Tensile Deformation and Failure Behavior of Single-Crystal $\beta$ -Sn

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## Abstract

Lead-free solder, particularly  $\beta$ -Sn, is critical for maintaining the structural integrity and functional reliability of integrated circuits. Understanding the mechanical properties and fracture behavior of  $\beta$ -Sn is therefore of great significance. In this study, molecular dynamics simulations using the modified embedded atom method were conducted to explore the mechanical properties and crack propagation of single-crystal  $\beta$ -Sn under varying strain rates. The results reveal that with increasing strain rates, single-crystal  $\beta$ -Sn exhibits higher yield strength, fracture strength, and fracture strain, accompanied by a decrease in elastic modulus. At elevated strain rates, pronounced strain hardening occurs due to a significant increase in internal dislocation density, which inhibits plastic deformation. These findings provide atomic-level insights into the strain-hardening mechanism and enhance the understanding of the mechanical behavior of single-crystal  $\beta$ -Sn. This study offers valuable guidance for optimizing the design and application of lead-free solder materials in the electronics industry.

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