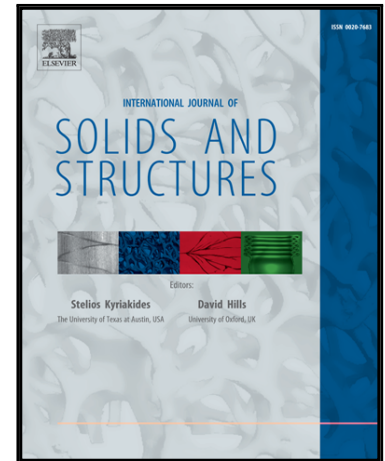


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Experimental and numerical investigations on stress induced phase transitions in silicon

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Abstract

Silicon has a tremendous importance as an electronic, structural and optical material. Modeling the stress driven phase transitions during the interaction of a silicon surface with a pointed asperity at room temperature is a major step towards the understanding of various phenomena related to brittle as well as ductile regime machining of this semiconductor. In order to understand the material's response for complex loading situations the often used J_2 -plasticity model is inadequate, instead dedicated constitutive models are required. We developed a novel finite deformation constitutive model set within the framework of thermodynamics with internal variables that captures the stress induced semiconductor-to-metal ($\text{cd-Si} \rightarrow \beta\text{-Si}$), metal-to-amorphous ($\beta\text{-Si} \rightarrow \text{a-Si}$) as well as amorphous-to-amorphous ($\text{a-Si} \rightarrow \text{hda-Si}$, $\text{hda-Si} \rightarrow \text{a-Si}$) transitions. The model was calibrated using load-displacement data for (111)-Si, which we show to be representative for the Berkovich indentation response of silicon. The simulation results for the residual surface topography and the size of the transformed zone agree very well with experimental data. Finally, the predictive capability of the model is demonstrated by the successful reproduction of the load displacement curve for indentation with the Knoop indenter tip. A comparison between residual stress fields computed using the phase transition model to results obtained using J_2 -plasticity shows significant differences, suggesting that predictions based on the latter may be unreliable.

Keywords: silicon, constitutive model, stress induced phase transition, indentation, contact loading

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