Liu, D. S.; **Tsai, C. Y.**

Estimation of thermo-elasto-plastic properties of thin-film mechanical properties using MD nanoindentation simulations and an inverse FEM/ANN computational scheme. (English)

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Summary: Utilizing a thin copper substrate for illustration purposes, this study presents a novel numerical method for extracting the thermo-mechanical properties of a thin-film. In the proposed approach, molecular dynamics (MD) simulations are performed to establish the load-displacement response of a thin copper substrate nanoindented at temperatures ranging from 300∼1400 K. The load data are then input to an artificial neural network (ANN), trained using a finite element model (FEM), in order to extract the material constants of the copper substrate. The material constants are then used to construct the corresponding stress-strain curve, from which the elastic modulus and the plastic level of the thin copper film are subsequently derived. The results show that both the elastic modulus and the plastic level decrease more than 30% as the simulation temperature increases from 300 K to 900 K. Comparing the result obtained from the ANN scheme for the elastic modulus of the thin copper film at room temperature with that obtained experimentally from a micro-force indentation test, it is found that the numerically-derived value (174 GPa) is higher than that obtained experimentally (145 GPa). The discrepancy between the two sets of results is thought to arise primarily as a result of the high strain rate employed in the MD simulations and the assumption of a perfect, defect-free monocrystalline copper microstructure.

MSC:

74C05 Small-strain, rate-independent theories of plasticity (including rigid-plastic and elasto-plastic materials)
74F05 Thermal effects in solid mechanics
74S05 Finite element methods applied to problems in solid mechanics
74K35 Thin films
74S30 Other numerical methods in solid mechanics (MSC2010)
92B20 Neural networks for/in biological studies, artificial life and related topics

Keywords:

thin film; thermo-mechanical properties; molecular dynamics (MD); artificial neural network (ANN); finite element method (FEM)

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