



Special Issue Reprint

Numerical Modeling of Materials under Extreme Conditions

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In this reprint, the underlying damage mechanisms of materials used under extreme conditions are explored using computer simulation and modelling methods, presenting important information to predict the lifetime of related facilities. The scope of this reprint embraces numerical work on material responses to extreme conditions, such as high-speed impact or loading, neutron or ion irradiation, and high-pressure and/or high-temperature environments. Related simulation results based on the first principle method, molecular dynamics, and finite element methods are reported. Results of various topics have been reported by papers collected in this book, for example, including fitting a better empirical potential, diffusion of atoms on surface, corrosion, interaction between different defects, elastic constants calculations, effect of hot press forming on collision toughness and energy distribution, and influence of radiation defects on the thermo-mechanical properties of UO2. Furthermore, a review about the experiments and models for the effect of strain rate on NiTi shape memory alloys (SMAs) has also been included in this reprint. These new results present new knowledge for understanding the damage mechanisms of materials under extreme conditions, which would be useful not only for researchers in these fields but also for new readers to learn about basic concepts and current research progress to better understand the response of materials under extreme conditions.



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