First Principles Modelling of Shape Memory Alloys: Molecular Dynamics Simulations (Springer Series in Materials Science)

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Materials sciences relate the macroscopic properties of materials to their microscopic structure and postulate the need for holistic multiscale research. The investigation of shape memory alloys is a prime example in this regard. This particular class of materials exhibits strong coupling of temperature, strain and stress, determined by solid state phase transformations of their metallic lattices.
The present book presents a collection of simulation studies of this behaviour. Employing conceptually simple but comprehensive models, the fundamental material properties of shape memory alloys are qualitatively explained from first principles. Using contemporary methods of molecular dynamics simulation experiments, it is shown how microscale dynamics may produce characteristic macroscopic material properties.
The work is rooted in the materials sciences of shape memory alloys and covers thermodynamical, micro-mechanical and crystallographical aspects. It addresses scientists in these research fields and their students.

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