First principles modelling of shape memory alloys : molecular dynamics simulations

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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.