Oliver Kastner

Molecular-dynamics of a 2D model of the shape memory effect
Part II: thermodynamics of a small system

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Abstract
This work investigates the thermodynamic properties of a qualitative atomistic model for austenite–martensite transitions. The model, still in 2D, employs Lennard-Jones potentials for the determination of the atomic interactions. By use of two atom species it is possible to identify three stable lattice structures in 2D, interpreted as austenite and two variants of martensite. The model is described in the first part of the work [6] in detail. The present work studies the thermodynamic properties of the model concerning a small, 2-dimensional test assembly consisting of 41 atoms. The phase stability is investigated by exploitation of the condition of minimal free energy. The free energy is calculated from the thermal equation of state, which is measured in numerical tensile tests. In the second part of this work a chain of eleven 41-atom assemblies is investigated. The chain is interpreted as an idealized larger body, where the individual crystallites represent crystallographic layers allowing for the creation of micro structure. By use of tensile tests at various temperature conditions we sketch how such chain may exhibit quasi-plasticity, pseudo-elasticity and the shape memory effect.

Keywords Molecular dynamic simulation · Solid-solid phase transitions · Phase stability · Martensitic transformation · Shape memory alloys

1 Introduction

1.1 Lattice transitions in Lennard–Jones solids

This work investigates the thermodynamic properties of an atomistic model for austenite–martensite phase transformations. The model was introduced in a preceding work [6]. It is restricted to two dimensions and employs Lennard–Jones potentials. The model rationalizes the characteristic properties of martensitic transformations qualitatively: mass points considered as atoms of two different species are placed in a symmetric, square lattice which represents austenite. Under the influence of temperature or load this lattice transfers into sheared variants of lesser symmetry, which represent variants of martensite. The atomic interaction parameters may be adjusted in a range, such that phase transitions between austenite and variants of martensite can be observed using molecular dynamic (MD) simulations. The phase stability then depends on the temperature, or on loads exerted.
The model has been tested qualitatively with small, two-dimensional crystallites of up to a few hundred atoms. Figure 1 shows eight snapshots of an unloaded 230-atom assembly during a MD simulation experiment under temperature control. Martensite and austenite are stable at low and high temperature, respectively. Austenite–martensite transformations \((a \rightarrow m)\) occur upon cooling from the austenitic regime and the reverse transformation \((m \rightarrow a)\) occurs upon heating from martensitic regime. If the temperature is cycled between values above and below the critical temperatures \(T_{c}^{a \rightarrow m}\) and \(T_{c}^{m \rightarrow a}\), a transition cycle like the one shown in Fig. 1 is observed. Austenite need not necessarily transform uniformly into martensite. Rather variants of martensite may be created indicated by different shear directions. Figure 2 shows a 298-atom assembly creating lattice layers with alternating shear directions upon cooling, interpreted as martensitic twins.

Fig. 1 a→m cycle of an unloaded 230-atom assembly under temperature control. \(T_{c}^{a \rightarrow m}\) and \(T_{c}^{m \rightarrow a}\) indicate transition temperatures.

Fig. 2 Micro-twin structure created by cooling a 298-atom assembly, which initially was austenitic.