TU Delft

Delft University of Technology

# Molecular dynamics simulations of phase transformations in niti bicrystals

Srinivasan, Prashanth; Nicola, Lucia; Simone, Angelo

**Publication date**
2016

**Document Version**
Final published version

**Published in**
Proceedings of the 24th International Congress of Theoretical and Applied Mechanics

**Citation (APA)**
Srinivasan, P., Nicola, L., & Simone, A. (2016). Molecular dynamics simulations of phase transformations in niti bicrystals. In J. M. Floryan, V. Tvergaard, & D. van Campen (Eds.), *Proceedings of the 24th International Congress of Theoretical and Applied Mechanics: 21-26 August 2016, Montreal, Canada* (pp. 1-2)

**Important note**
To cite this publication, please use the final published version (if applicable).
Please check the document version above.

**Copyright**
Other than for strictly personal use, it is not permitted to download, forward or distribute the text or part of it, without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license such as Creative Commons.

**Takedown policy**
Please contact us and provide details if you believe this document breaches copyrights.
We will remove access to the work immediately and investigate your claim.

*This work is downloaded from Delft University of Technology.*
*For technical reasons the number of authors shown on this cover page is limited to a maximum of 10.*

# MOLECULAR DYNAMICS SIMULATIONS OF PHASE TRANSFORMATIONS IN NITI BICRYSTALS

Prashanth Srinivasan *[1], Lucia Nicola[2], and Angelo Simone[1]
[1]*Faculty of Civil Engineering and Geosciences, Delft University of Technology*
*Delft, The Netherlands*
[2]*Faculty of Mechanical, Maritime and Materials Engineering, Delft University of Technology*
*Delft, The Netherlands*

*Summary* The influence of grain boundaries and grain misorientation on the nucleation and growth of martensite in an equi-atomic nickel-titanium (NiTi) shape memory alloy (SMA) is investigated by performing molecular dynamics (MD) simulations on bicrystals with a modified embedded atom method (MEAM) interatomic potential. Stress-induced martensitic transformations are simulated in bicrystals with mixed grain boundaries and the behavior of the bicrystal is compared to that of individual single crystals. Here, a particular bicrystal with $< 110 >$ and $< 111 >$ oriented austenite grains is chosen as an example. Results indicate that the mixed grain boundary in the austenite bicrystal acts as a nucleation site for stress-induced martensitic transformation in the grains. The deformation behavior and the transformation strain of the bicrystal fall in between those of the two corresponding single crystals.

## INTRODUCTION

SMAs can exist in different phases depending on temperature and stress. This leads to interesting properties such as pseudo-elasticity and the shape memory effect. The reversible phase transformation happens between a high-symmetry B2 austenite phase, stable at high temperatures, and a low symmetry B19' martensite phase, stable at low temperatures. Under the application of a load at high temperatures, the austenite phase undergoes large reversible deformations up to a strain of 10 % by transforming into the martensite phase. This transformation is very sensitive to grain orientation [1], grain size [2] and grain boundaries (GBs) [3, 4, 5] which are known to influence the nucleation of martensite, the transformation stress and strain, and the type of variant in regions near the grain boundary. Since the martensitic transformation occurs rapidly, it is difficult to understand the precise role of various types of grain boundaries by performing experiments. This is why molecular dynamics is an important tool in understanding the underlying micro-structural changes during such phase transformations. So far, MD has been limited to study temperature and stress-induced transformations in single-crystal NiTi [6, 7]. In this work, we study the influence of mixed grain boundaries on stress-induced martensitic transformations by simulating differently oriented NiTi bicrystals.

## METHODOLOGY

A specific bicrystal with a mixed high-angle grain boundary is chosen as an example to discuss method and results. A 3-D cell with periodic boundary conditions along all directions consisting of two grains of different orientation (Fig. 1(a)) is used. Overlapping atoms near the GB that are very close to each other are deleted. The two GBs, one in the middle of the cell and

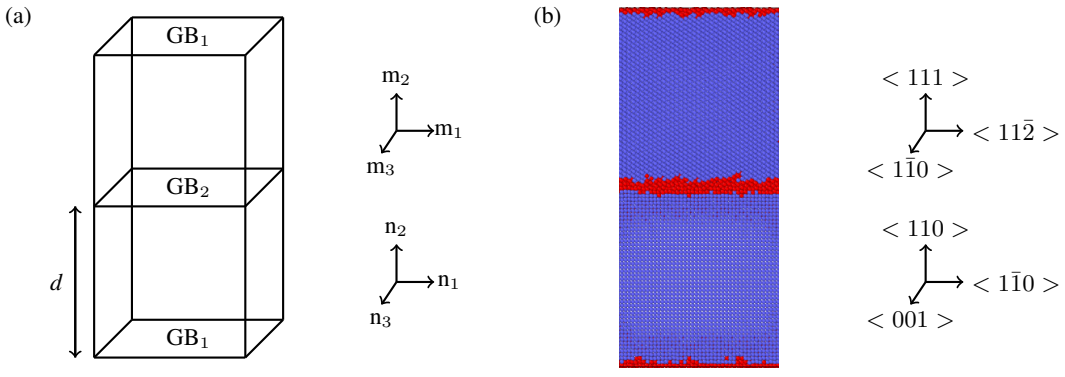


Figure 1: (a) Schematic of the 3-D periodic bicrystal simulation cell. (b) Sectional view of a relaxed bicrystal with a mixed grain boundary (atoms in red); orientation of individual grains is also shown.

*Corresponding author. Email: P.Srinivasan@tudelft.nl

one that arises because of periodicity are similar and the separation $d$ between them is large enough to independently study the effect of the GB. In this work, we choose $d$ =15 nm and 15 nm $\times$ 15 nm $\times$ 15 nm grains. The initial structure is austenite with the orientation of the two grains shown in Fig. 1(b).

An energy minimisation is performed to obtain the minimum energy GB structure. After that, the bicrystal is allowed to thermally equilibrate at 350 K. The loading axis is perpendicular to the GB plane. Tensile and compressive loading simulations are performed at a strain rate of $10^7$ $s^{-1}$. To compare results with single crystal behaviour, bulk single crystals along $< 110 >$ and $< 111 >$ axis are subjected to the same boundary conditions. All simulations are performed with LAMMPS using the MEAM interatomic potential [8].

## RESULTS AND DISCUSSION

Figure 2 shows the tensile (a) and compressive (b) stress-strain response of the B2 bicrystal shown in Fig. 1(b) and that of the individual single crystals loaded along the $< 110 >$ and $< 111 >$ axis at 350 K. In all cases, there are two regions of linear deformation, corresponding to phases B2 and B19', that are separated by a non-linear region – this implies the transformation and leads to super-elasticity. The stiffness of B2 and B19' and the strain associated with the stress plateau for the bicrystal are in between the corresponding single crystal values. Under both tension and compression, the GB acts as a nucleation site for the onset of martensitic transformation, starting in the bottom grain in Fig. 1(b). In this particular bicrystal, the GB does not affect martensite variant selection since the same variants are formed in each grain and in the individual single crystals (results not shown here).

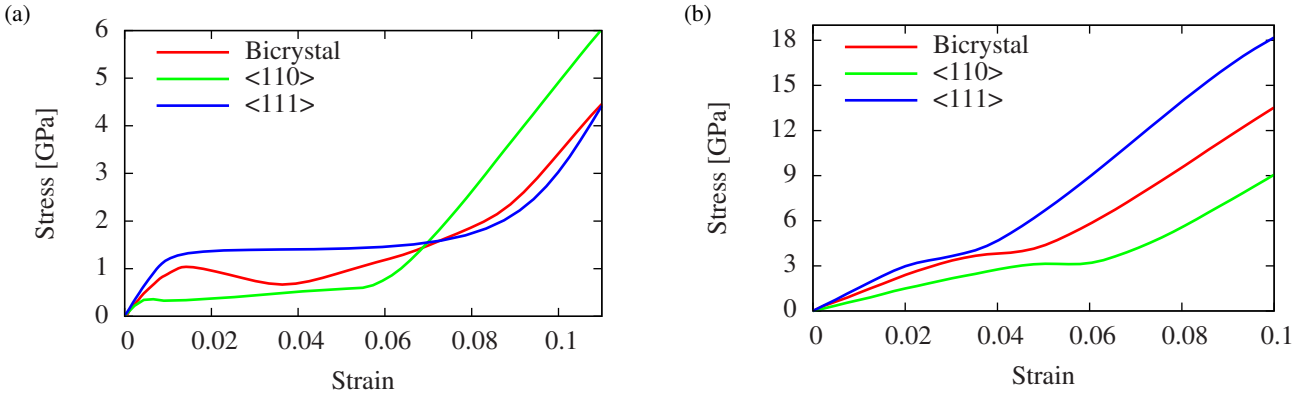


Figure 2: Isothermal stress-strain behavior of the bicrystal in Fig. 1(b) compared to individual bulk single crystals at 350 K under (a) tension and (b) compression.

## References


[1] Pfetzing-Micklich J., Somsen C., Dlouhy A., Begau C., Hartmaier A., Wagner M.F.X., Eggeler G.: Acta Mater. **61**, 602-616 (2013).
[2] Waitz T., Spisak D., Hafner J., Karnthaler H.P.: Europhys. Lett. **71**, 98-103 (2005).
[3] Ueda M., Yasuda H., Umakoshi Y.: Science and Tech. of Adv. Mat. **3**, 4-9 (2002).
[4] Ueland S.M., Schuh C.A.,: J. App. Phys. **114**, 053503 (2013).
[5] Kato H., Miura S.: Mat. Sci Forum **394-395**, 205-208 (2002).
[6] Mutter D., Nielaba P.: European Phys. J. **84**, 109-113 (2011).
[7] Zhong Y., Gall K., Zhu T.: J. App. Phys. **110**, 033532 (2011).
[8] Ko W-S., Grabowski B., Neugebauer J.: Phys. Rev. B. **92**, 134107 (2015).