AMTC Letters
Vol. 1 (2008)

A Way from nano-scale Molecular Dynamics to the macro-scale Study of Damping Capacity of Ti-Ni Shape Memory Alloy.

Tetsuro Suzuki

Research Staff, National Institute for Materials Scienence, Tsukuba 305-0047, Japan.

Molecular Dynamics (MD) based on the Parrinello-Rahman scheme have been used to study wide range of materials properties if a proper inter-atomic potential is available for the materials to be investigated. We have shown that a simple 8-4 Lennard-Jones potential allows us to simulate the martensitic transformation in the Ti-Ni shape memory alloys which have been recently attracting attention as materials for damping wide frequency range of vibrations and noises. MD is powerful if the materials properties of interest are governed with the behaviors in nano-scales. But if they are governed with those in macro-scale, MD needs a way out of the limitation imposed by the computing power of even the most powerful facilities. The purpose of the present poster presentation is to show a way out of this limitation for the calculation of the damping capacity in the Ti-Ni shape memory alloy by use of scaling scheme proposed by the random filed Ising spin model.

The presence of twin boundaries, which can exist only in the low temperature phase, i.e. the martensitic phase, are responsible for the shape memory effect as well as high damping capacity in Ti-Ni alloys. Experimentally it has been established that the prominent characteristic of the damping capacity is its dependence on the amplitude of externally applied cyclic stress, i.e. the higher damping the higher amplitude. The mechanism for the damping associated with the twin boundaries as 2-dimensional lattice defects is entirely different from that associated with dislocations as 1-dimensional lattice defects. While in the former dependence on the amplitude of applied stress comes from the inevitable hysteresis motion of twin boundaries, in the latter the corresponding dependence must comes from the breakaway of dislocation lines from their impurity pinning points: a rather complicated mechanism for damping.

Because the stress required to move entire twin boundaries in a macroscopic crystal is very large compared with the amplitude of cyclic stress, the breakaway of dislocation lines, which are supposed to constitute twin boundaries, have been adopted as the established method to analyze the damping capacity. However, the proposition that twin boundaries are constituted of dislocation arrays is hard to be justified, because the twin boundaries have irrational crystal indices.

We initiated the investigate the temperature dependence of damping capacity by use of MD without

assuming any model for twin boundaries in the martensitic phase of Ti-Ni alloy and obtained the hysteresis loss as shown in Fig.1. Also we investigated the damping capacity in Ti-Ni alloy, which contains 4% of vacancies as a model for various point defects also shown in Fig.1. Here, we notice that calculated temperature dependence of the damping capacity by MD is not in agreement with experimental results in the temperature where the martensitic phase has finished its formation. However, MD can reproduce the recent experimental results, where the normal martensitic transformation is suppressed by the introduction of high concentration of lattice defects, where an extrinsic scale imposed by the presence of lattice defects turns out smaller than MD cell size.

The scheme based on the random field Ising spin model as shown in Fig.2 proposes that the relationship like the stress-strain relationship which gives the damping capacity in the nano-scale can be translated to the corresponding one in the macro-scale. This is a way to utilize the results of the nano-scale MD calculation to obtain the damping capacity in macro-scale materials.

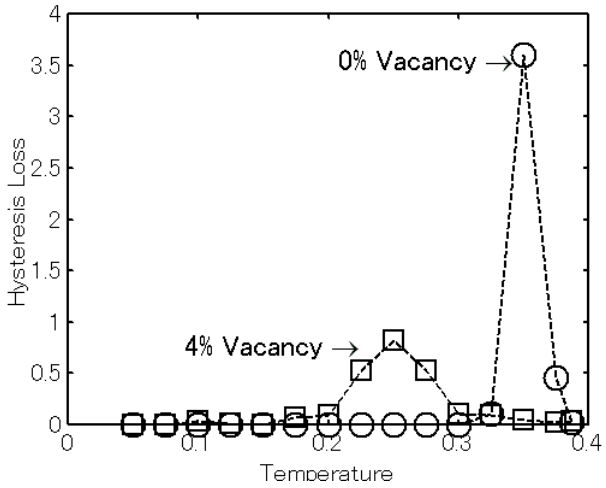

FIG.1 Temperature dependence of the damping capacity calcluated by molecular dynamics as hysteresis loss for cyclic stress in the model crystals with and without vacancies as models for point lattice defects.---

$$s_i' = Ns_i$$

$$H'N = H$$
$$r'(i,R')N = r(i,R)$$
$$J'N^2 = J$$

$$\mathrm{H} = -\sum_i \sum_j Js_i s_j - \sum_i (r(i,R)s_i + Hs_i)$$

$$\mathrm{H}' = -\sum_i \sum_j J's_i's_j' - \sum_i (r'(i,R)s_i' + H's_i')$$
$$= -\sum_i \sum_j J'N^2 s_i s_j - \sum_i (r'(i,R)Ns_i + H'Ns_i)$$

$$\oint H' d\left(\sum_i s_i'\right) = \oint \frac{H}{N} d\left(\sum_i Ns_i\right) = \oint H d\left(\sum_i s_i\right)$$

FIG.2 Hysteresis loss at different scale is related in the scheme proposed by the random field Ising spin model .