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The unified mechanism of aging effects in both martensite and parent phase for shape-memory alloys: atomic-level simulations J. DENG, X. DING, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China, T. SUZUKI, K. OTSUKA, Ferroic physics Group, National Institute for Materials Science, Tsukuba 305-0047, Ibaraki, Japan, T. LOOKMAN, A. SAXENA, Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA, J. SUN, State Key Laboratory for Mechanical Behavior of Materials, Xi'an Jiaotong University, Xi'an 710049, China, X. REN, Ferroic physics Group, National Institute for Materials Science, Tsukuba 305-0047, Ibaraki, Japan — Most shape-memory alloys (SMAs) subject to the aging effects not only in the martensite phase but also in the parent phase. These aging effects have been attracted much attention as they strongly affect the practical applications of SMAs. So far, the intrinsic mechanism of them has remained controversial due to the difficulty in visualization of what happens in atomic scale. In the present study, by using a combination of molecular dynamics method and Monte-Carlo method [1], we investigate the aging effects in both martensite and parent phase. We successfully reproduced the thermal behaviors of aging effects for SMAs, i.e., the A_f temperature increase with aging time in martensite and the M_s temperature decrease with aging time in parent phase, which keep good agreement with the experimental observations [2]. In addition, quantitative analysis of the atomic configurations during aging reveals that the aging effects are not associated with a change in the average structure.

Junkai Deng
State Key Laboratory for Mechanical Behavior of Materials,
Xi'an Jiaotong University, Xi'an 710049, China

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