*Supplementary*

# Molecular Dynamics Investigation on Grain Size-Dependent Superelastic Behavior of CuZr Shape Memory Alloys

**Mixun Zhu [1], Kai Wang [1], Hongtao Zhong [1], Huahuai Shen [1], Yong Zhang [2], Xiaoling Fu [1,*] and Yuanzheng Yang [1,*]**

[1] School of Materials and Energy, Guangdong University of Technology, Guangzhou 510006, China; zhumixun@163.com (M.Z.); 15917162027@163.com (K.W.); zht790319109@163.com (H.Z.); shenhh2020@126.com (H.S.)
[2] Beijing Advanced Innovation Center of Materials Genome Engineering, State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, 30 Xueyuan Road, Beijing 100083, China; drzhangy@ustb.edu.cn
* Correspondence: fuxiaoling@gdut.edu.cn (X.F.); yangyz@gdut.edu.cn (Y.Y.)

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## Supplementary Note 1

This section presents the shear strain distribution and phase configuration of a polycrystalline B2-CuZr sample with a grain size of 6.59 nm at the critical strain for martensitic transformation ($\varepsilon$ = 0.0215), as shown in Figure S1. It can be observed that the green regions of high shear strain within the grain interior correspond to the locations of the R phase, as highlighted by the red circles in Figure S1.

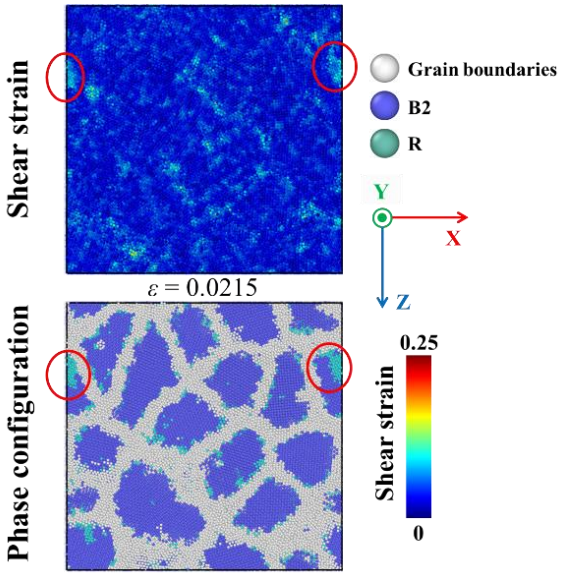



**Figure S1.** The shear strain and phase configuration of the polycrystalline B2-CuZr sample with a grain size of 6.59 nm at the critical strain for martensitic transformation ($\varepsilon$ = 0.0215).

## Supplementary Note 2

This section presents the shear strain distribution and phase configuration of a polycrystalline B2-CuZr sample with a grain size of 6.59 nm at the maximum loading strain ($\varepsilon$ = 0.08), as shown in Figure S2. In Figure S2, white circles denote the R phase, while black circles represent the B2 phase. It can be observed that the green regions of high shear strain within the grain interior correspond to the locations of the R phase, while the blue regions of low shear strain correspond to the untransformed B2 phase.

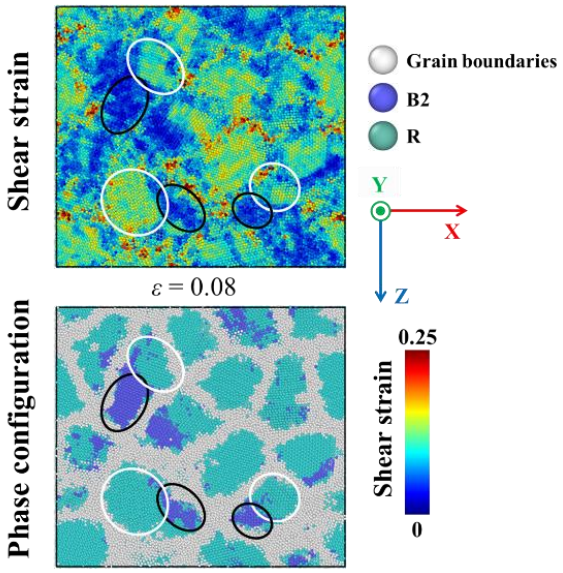



**Figure S2.** The shear strain and phase configuration of the polycrystalline B2-CuZr sample with a grain size of 6.59 nm at the maximum tensile strain ($\varepsilon = 0.08$).