Electronic Supplementary Material (ESI) for Nanoscale.

Nonuniform-to-Uniform Structural Transition Induced by Ultrasonic Vibration

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Supplementary Material

Section 1: Configurations of the Mg-Al nanolayers before their joining processes

Figure S1 shows the configurations of all Mg-Al nanolayers before their joining processes, with each obtained via the four steps given in the section "METHODS". Since a higher T_e leads to a longer time of the heating step according to the step (ii), the motion of atoms are more activated at a higher T_e. Thus, the thickness of the slightly-mixed interface varying from 1-atom to about 2-atom layer as the T_e increases. Although these differences would lead to differently final thicknesses of the interfaces at different T_e, it would not interfere with comparing results between the two distinct joining methods to access the role of UV in determining the structural evolution of the Mg/Al interface.

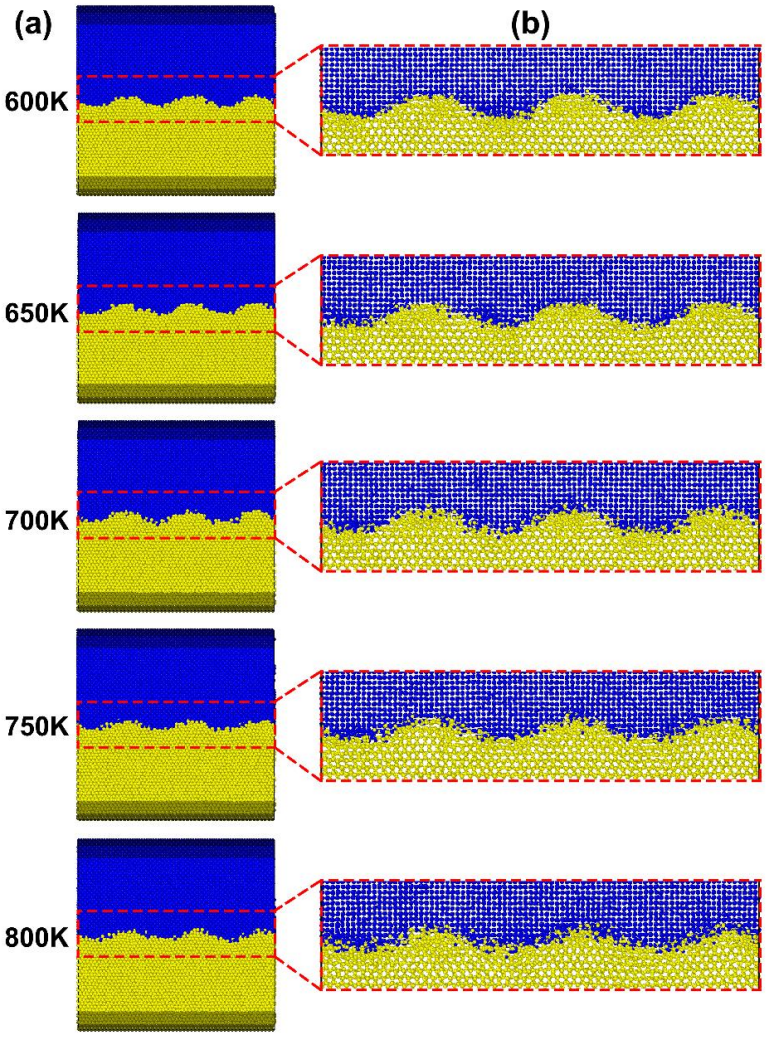

Figure S1. The configurations of the Mg-Al nanolayers before their joining processes. Mg atoms are yellow and Al atoms are blue.

Section 2: The joining processes of the Mg-Al nanolayers at different T_e

Figure S2 shows that, as the diffusion time increases from 0 to 5 ns, the Mg/Al interface at each T_e still maintains in a wave-like shape in the case free of UV, but gradually changes into a slab-like and more uniform one in the case with UV, revealing that the applied UV can lead to a nonuniform-to-uniform transition in the structure of the joined Mg/Al interface in the Mg-Al nanolayer.

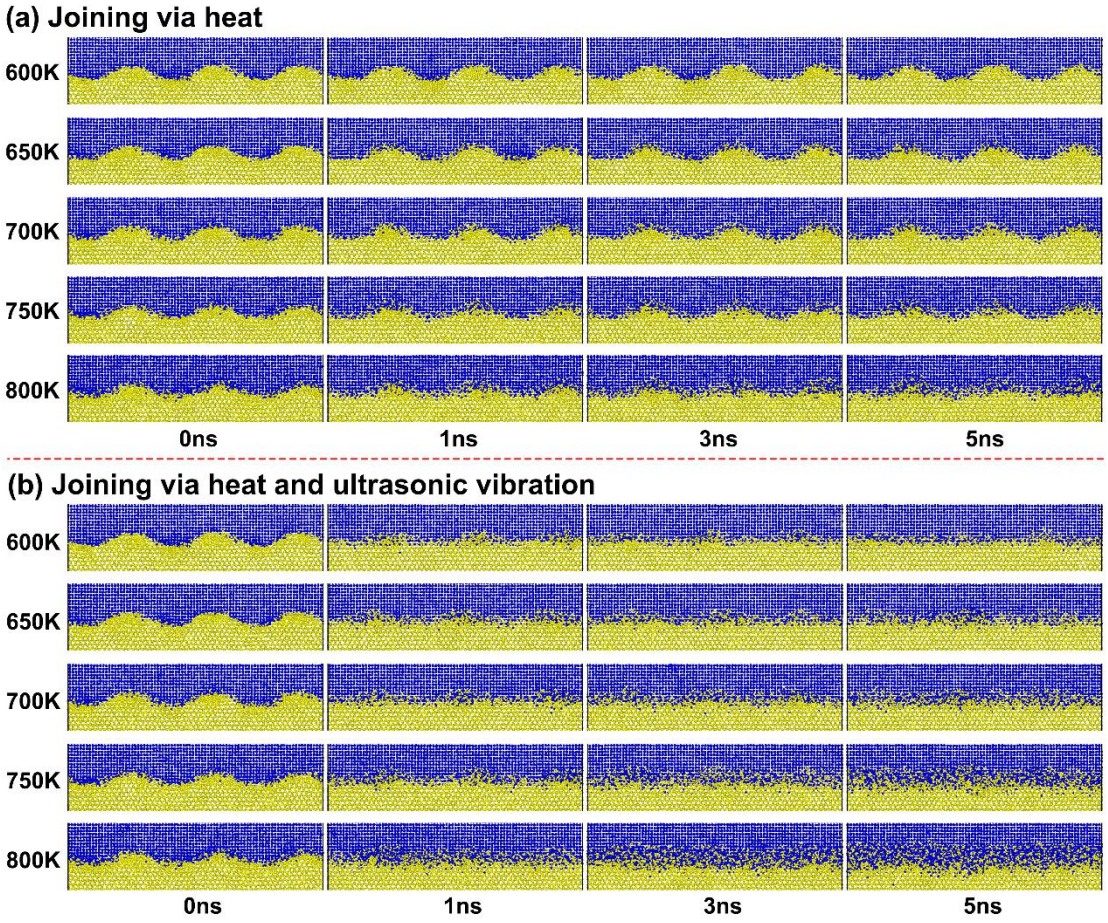

Figure S2. The joining of the Mg-Al nanolayers by (a) heat and (b) heat and ultrasonic vibration. In the case with UV, B=5 nm and f=5.7 GHz.

Section 3: The distributions of defect meshes of the Mg-Al nanolayers

Figure 3S presents the structural analysis profiles of the free layers of the Mg-Al nanolayers at all T_e. In the case free of UV, the h slightly changes as the diffusion time increases from 0 to 5 ns, meaning that it is difficult to break the structural equilibrium of the interface via heat-induced atomic diffusion, even though the system temperature is up to 800 K. This is because both sides of the Mg/Al interface keep in their initial FCC or HCP structures, only with the interface in an amorphous structural order, dramatically restricting atoms to move across the interface. This feature of the Mg/Al interface is quite different from other interfaces such as Cu/Al and Co/Zr interfaces [S1, S2]. At these interfaces, before any interdiffusion occurs, the Al (or Co) side has exhibited an amorphous structural order at or above a temperature (650 K for Al and 1620 K for Co) much lower than its melting point, facilitating Cu (or Zr) atoms to diffuse into the opposite side and consequently resulting in the increase in the thickness of the interface. However, in the case with UV, the final h markedly larger than the correspondingly initial one, and increases with the increasing T_e, meaning that the applied UV makes the thickness of the joined interface become thicker via enlarging the defect mesh of the jointed interface.

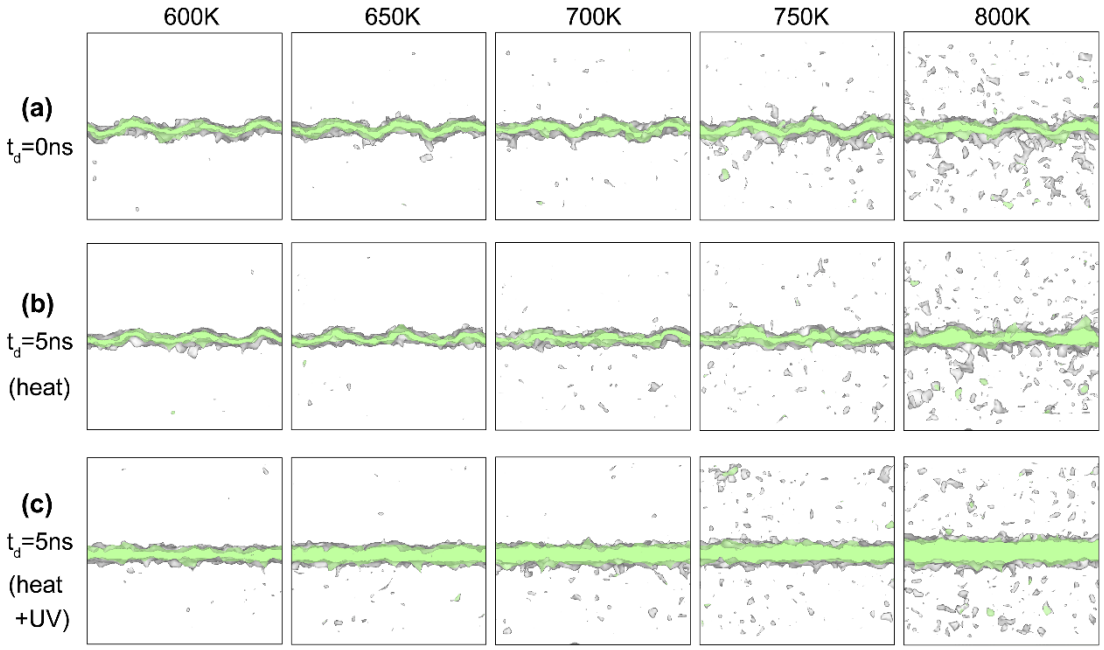

Figure S3. Distributions of defect meshes of the Mg-Al nanolayers. In the case with UV, B=5 nm and f=5.7 GHz.

REFERENCES

(S1) Chen S, Ke F, Zhou M, et al. Atomistic investigation of the effects of temperature and surface roughness on diffusion bonding between Cu and Al. Acta Materialia, 2007, 55(9): 3169−3175.

(S2) Weissmann M, Ramírez R, Kiwi M. Molecular-dynamics model of interface amorphization. Physical Review B, 1992, 46(4): 2577.