Coherent-Interface-Induced Second Hardening Deformation of Al-Mg-Al Nanolayers by Molecular Dynamics Simulations

Xue-Qi Lv[1,2], Xiong-Ying Li[3,*] Hong-Bing Liu[1,4]

[1]*School of Materials Engineering, Shanghai University of Engineering Science, Shanghai, 201620, China*

[2]*Shanghai Collaborative Innovation Center of Laser Advanced Manufacturing Technology, Shanghai, 201620, China*

[3]*College of Energy Engineering, Zhejiang University, Hangzhou 310007, China*

[4]*Shanghai Collaborative Innovation Center of Intelligent Manufacturing Robot Technology for Large Components, Shanghai, 201620, China*

Supplementary Material

Section 1: The Fabrications of Al-Mg-Al Nanolayers

The fabrication process includes four steps. Step 1 is the initial Al-Mg-Al nanolayer (Fig. S1a), in the dimension of xyz=153.967×45.391×72.946 $Å^3$ and with a layered thickness of about 22.7 Å (10080 Mg atoms and 15128 Al atoms), being relaxed at 300 K for 500 ps. Steps 2 and 3 are the nanolayer being heated from 300 K to the temperature T1 and cooled from T1 to 300 K, respectively. Twice changing rates of temperature are both 0.5 K/ps. T1 equals 300, 314, 440, 580, 650, or 664–846 K (at the intervals of 14 K). Step 4 is the nanolayer being kept at 300 K for 500 ps to optimize its structure. After these four steps, a series of energy-stable and jointed Al-Mg-Al nanolayers are obtained and possess two features. One feature is that the jointed Al/Mg interface is in different levels of jointing with respect to different T1. As T1 increases from 300 to 846 K, the thickness of the jointed area in Y direction gradually increases from 0 to 4 atomic layers (Fig. S1b). For example, in the case with T1=846 K, there are 4 peaks in the atomic density distribution curves, implying 4 atomic layers in each jointed interface (Fig. S1c). The other feature is that the radial distribution functions of the nanolayers in different cases of T1 (Fig. S1d) nearly coincide, with the positions of the first peaks for either Al atoms or Mg atoms varying over a small range (<0.015 Å), implying the similar crystal structures of Mg (or Al) layers in the nanolayers to that of pure Mg (or Al) crystal. This feature is beneficial to assess the effect of the jointed interface on the tensile deformation behavior of the nanolayers.

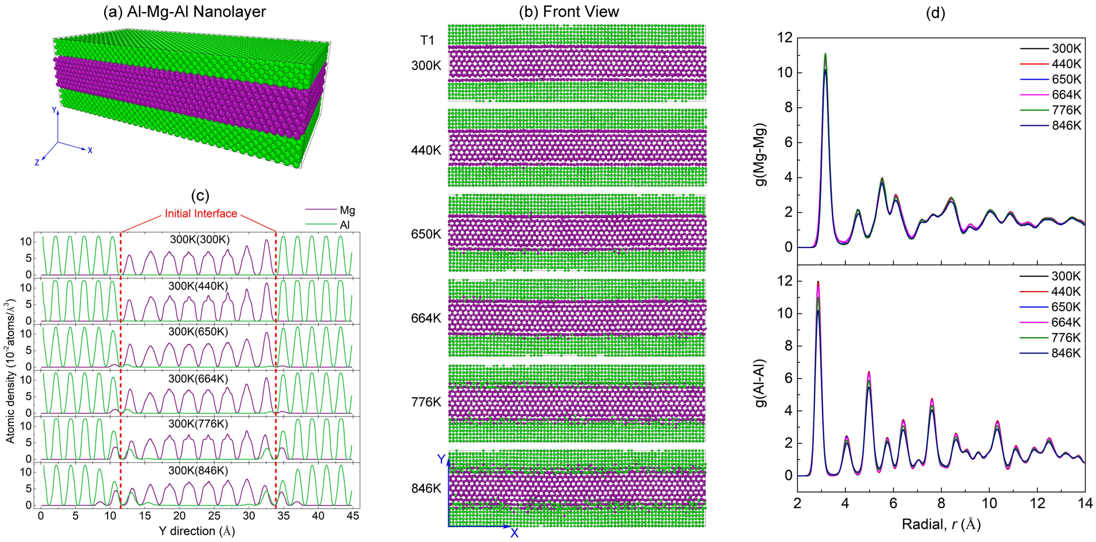

Figure S1. The structural profiles of the Al-Mg-Al nanolayers. (a) The initial configuration of the Al-Mg-Al nanolayer. (b), (c) and (d) are separately the final structures, atomic density distributions and radial distribution functions of the Al-Mg-Al nanolayers at the end of the step 4 in different cases of T1.

Section 2: The Tensile Behavior of The Al-Mg-Al Nanolayers in The Cases of Low Temperatures

Fig. S2 shows that the stress-strain curve of each Al-Mg-Al nanolayer in the cases of low temperatures (300≤T1<664 K) is quantitatively similar.

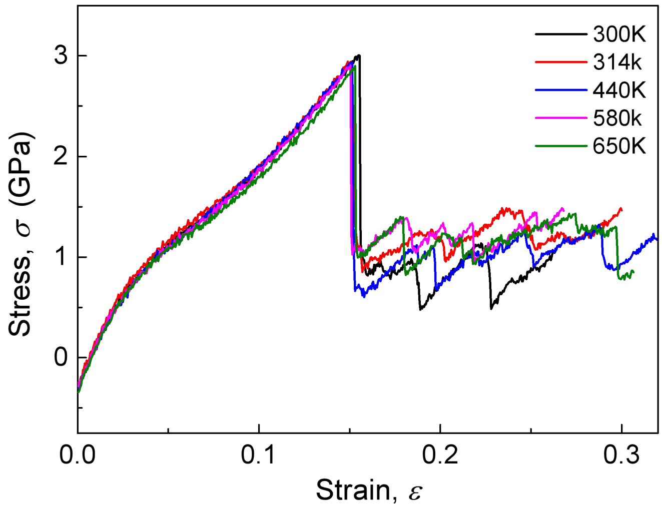

Figure S2. The stress-strain curves of the Al-Mg-Al nanolayers in the cases of low T1.

Section 3: The Tensile Behavior of The Al-Mg-Al Nanolayers in The Cases of High Temperatures

Fig. S3a shows that before the stress reaching the tensile strength, the nanolayers in all cases of high temperatures except for the cases with T1=692 and 748 K and response to the tensile strain with twice hardening deformations, between which a weak softening deformation with a small drop of about 0.3 GPa in the stress occurs at a point near the maximum-stress point. Fig. S3b displays that the Al-Mg-Al nanolayer in the case with T1=818 K possesses the best comprehensive tensile properties, with σ_b=3.03 GPa, ε_b=0.182 and a large stress of 2.27 GPa after the nanolayer fails.

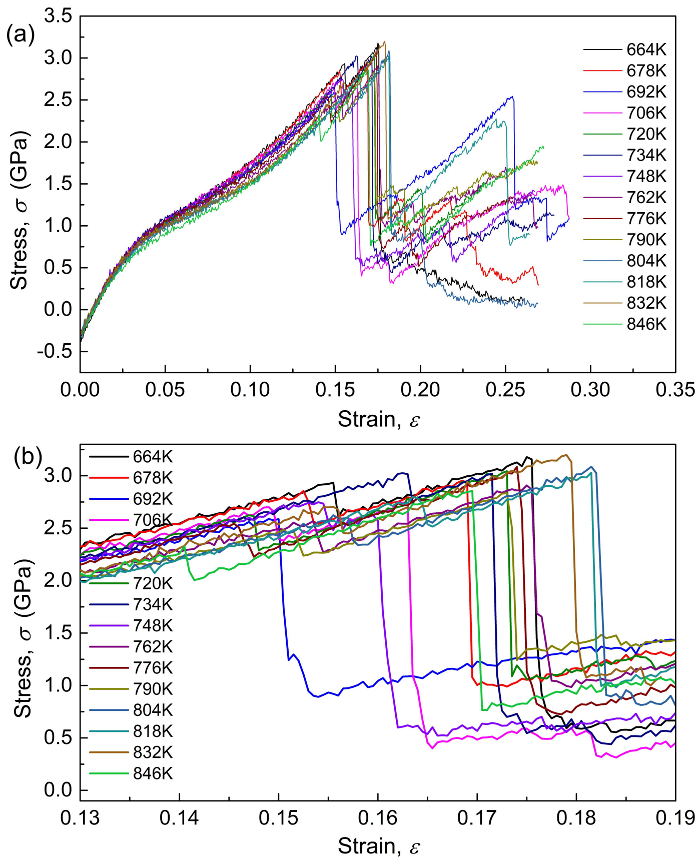

Figure S3. The stress-strain curves of the Al-Mg-Al nanolayers in the cases of high T1. (a) The complete stress-strain curves. (b) An enlargement of the stress-strain curves near the tensile strength.

Section 4: The Effect of Strain Rate on Tensile Behavior of Al-Mg-Al Nanolayers in the cases of high temperatures

In the cases of high temperatures (T1≥664 K), the formations of coherent Al/Mg interfaces are not observed at 2×10^9 and 2×10^{10} s^{-1}, as indicated by the stress-strain curves of the representative case of T1=734 K in Figure S4.

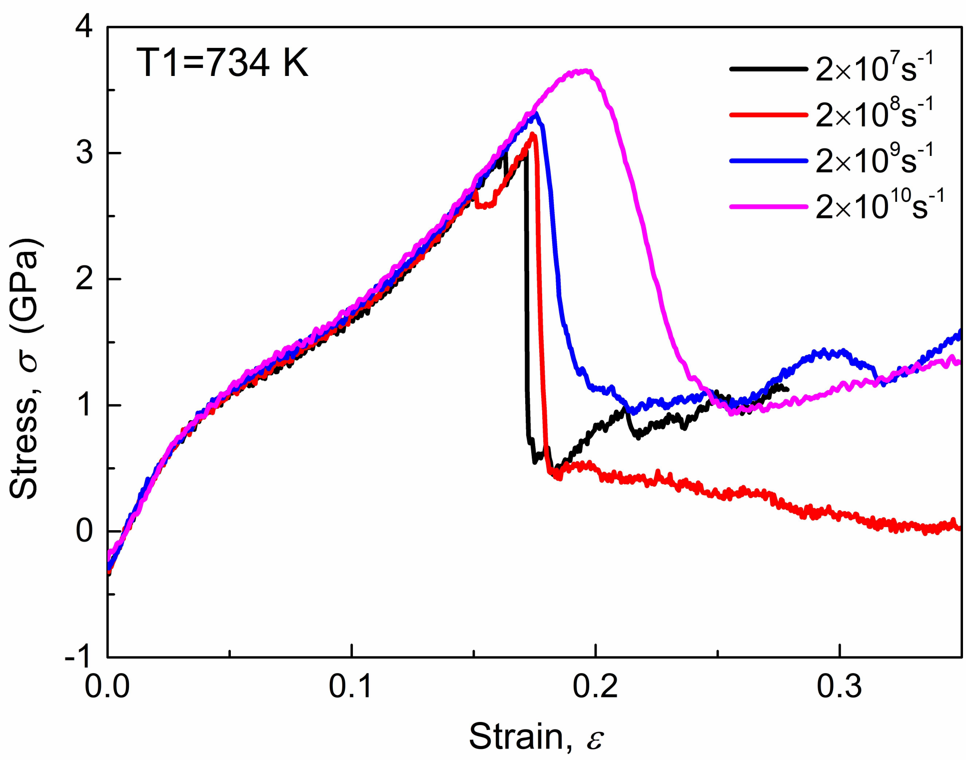

Figure S4. The stress-strain curves of the Al-Mg-Al nanolayers in the case of T1=734 K at different strain rates.