The valuable contribution of stress to the thermal stability of nanograined polycrystalline alloys

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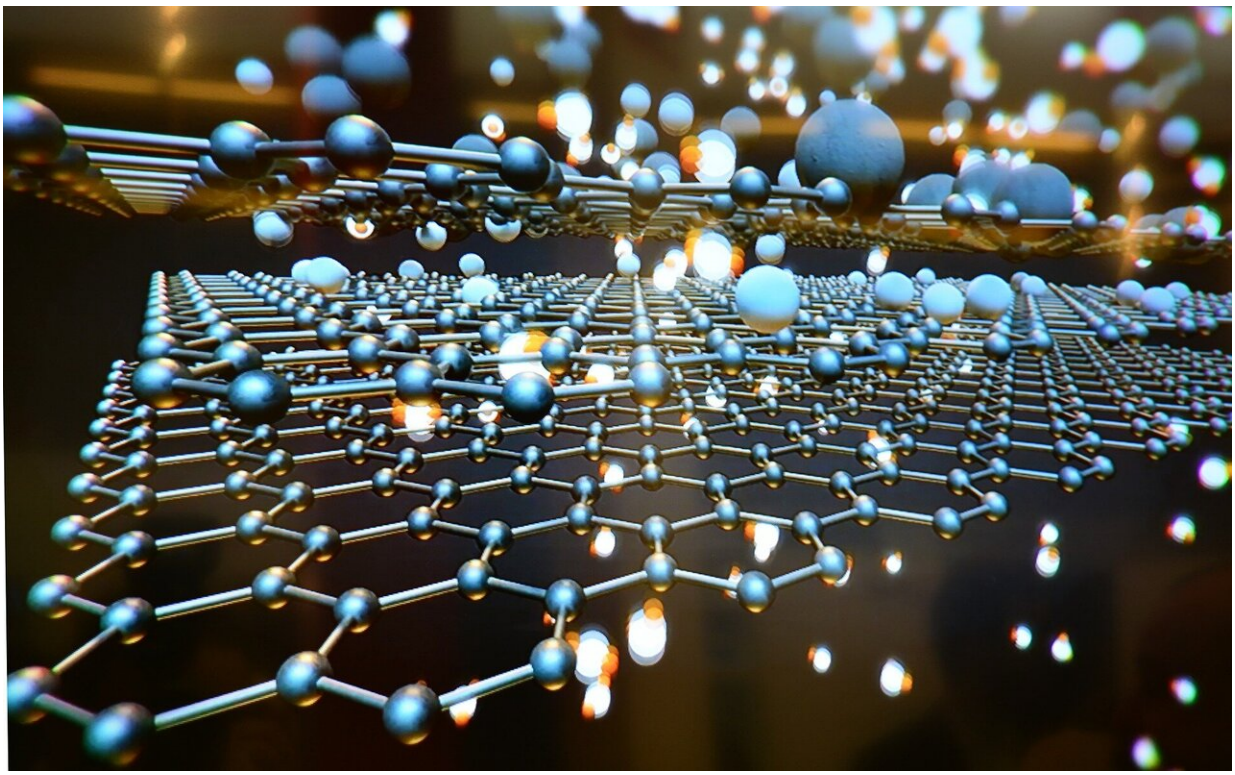

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Nanograined metals and alloys, whose grain size is less than 100 nm, exhibit extremely high strength and high ductility, possessing excellent mechanical properties. Nanograined materials, however, have a large

number of grain boundaries and hence high total grain boundary energy. At a temperature higher than a critical temperature, grains in nanograined materials will grow spontaneously to reduce the grain boundary energy, leading to thermal instability of the materials. A common approach to enhance thermal stability is via grain boundary energy segregation, which thermodynamically lowers the grain boundary energy and kinetically pins the movement of grain boundaries, thereby enhancing the critical temperature of recrystallization. However, the role of mechanical stresses in the thermal stability has not been systematically studied yet.

A recently published paper entitled "Grain boundary segregation and relaxation in nano-grained polycrystalline alloys," in *SCIENCE CHINA Physics, Mechanics & Astronomy*, systematically studies the thermal stability of nanograined alloys, by analytic investigation of three coupled behaviors between grain boundaries and crystalline grains among chemical concentrations and mechanical stresses. The three coupled behaviors are 1) the coupling between grain boundary stress and grain stress, 2) grain boundary segregation, and 3) the coupling between concentration and stress. Finally, a novel thermodynamic criterion is developed for the thermal stability of nanograined alloys, which shows stresses play an extremely role there. The authors of the paper are Zhang Tong-Yi, Gao Yingxin and Sun Sheng from Materials Genome Institute, Shanghai University.

The thermodynamic energy is divided into the mechanical energy and the chemical energy and both are coupled each other. The analysis of mechanical energy considers the grain boundary eigen-stress and the eigen-strain induced by grain boundary segregation and develops a hybrid method to solve the eigen-stress and eigen-strain coupling problem. The chemical thermodynamics analysis considers the difference in the chemical potentials of pure elements in grain boundaries and in grains, and hence proposes a generalized McLean

adsorption isotherm, which naturally includes the stress term. Based on the three coherent coupling effects, a novel criterion is developed for the thermal stability of nanograined alloys, and quantitatively and analytically expressed by the difference in molar free energy between a nanograined polycrystalline alloy and its single crystal counterpart. A positive or negative difference in molar free energy indicates the nanograined alloy is thermal unstable or stable.

Ni1-xMox binary alloys are taken as an example to illustrate, with figures, the theoretical results and the roles of each parameters involved in the analytic criterion. The present study shows that stresses play a vital role in the thermal stability of nanograined alloys. Any criteria without considering internal stresses would partially estimate the thermal stability of nanograined alloys.

More information: Tong-Yi Zhang et al, Grain boundary segregation and relaxation in nano-grained polycrystalline alloys, *Science China Physics, Mechanics & Astronomy* (2021). DOI: 10.1007/s11433-020-1614-5

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