Supplementary Information

Mechanical tensile response of Ni−graphene nanocomposites in hydrogen-irradiation coupled environments using molecular dynamics simulations

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Total Pages*:* 4 excluding cover pages

Total Figureures: 7

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1. Supplementary methodology

The coordinate system of single-crystal nickel model is oriented such that the x-, y-, and z-axes correspond to the [$\bar{1}$10], [$\bar{1}$ $\bar{1}$2], and [111] crystallographic directions, respectively. The system encompasses 100,000 Ni atoms, within a simulation cell of 124.2 × 86.0 × 101.5 Å^3 (see Figure. S1(a)). H atoms were subsequently incorporated at a designated concentration, as depicted in Figure. S1(b), using a randomized distribution scheme.

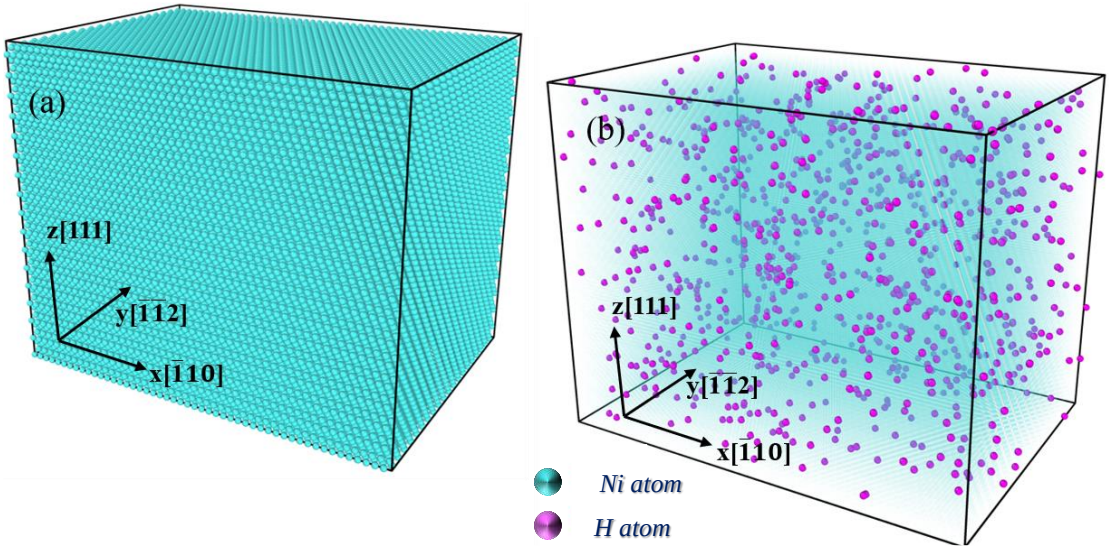

Figure S1. Computational model representations. (a) Initial atomic arrangement of the defect-free single-crystal nickel. (b) Atomic conFigureuration of the single-crystal nickel containing 10,000 appm of hydrogen.

2. Supplementary results

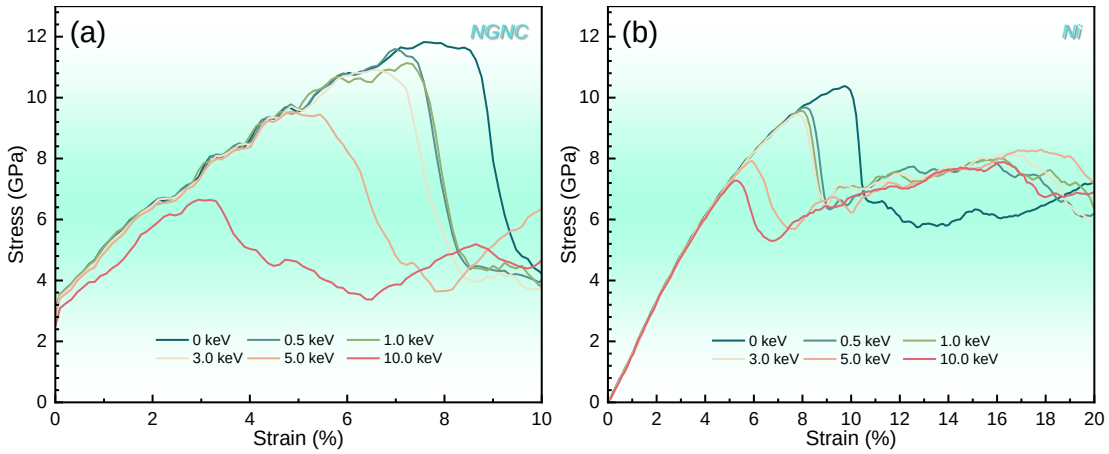

Figure S2. Engineering stress–strain curves measured at 300 K with a strain rate of 2×10^{-3} ps^{-1} in hydrogen-free environments, comparing different PKA energies. (**a**) NGNC. (**b**) Single-crystal nickel.

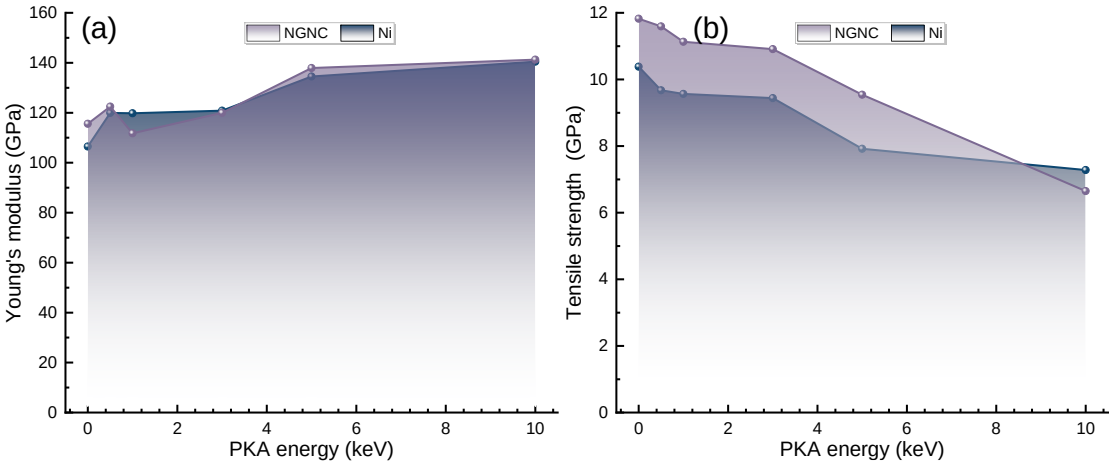

Figure S3. PKA energy dependence of mechanical parameters for NGNC and single-crystal nickel, measured at 300 K with a strain rate of 2×10^{-3} ps^{-1} in hydrogen-free environments. (**a**)Young's modulus. (**b**) Ultimate tensile strength.

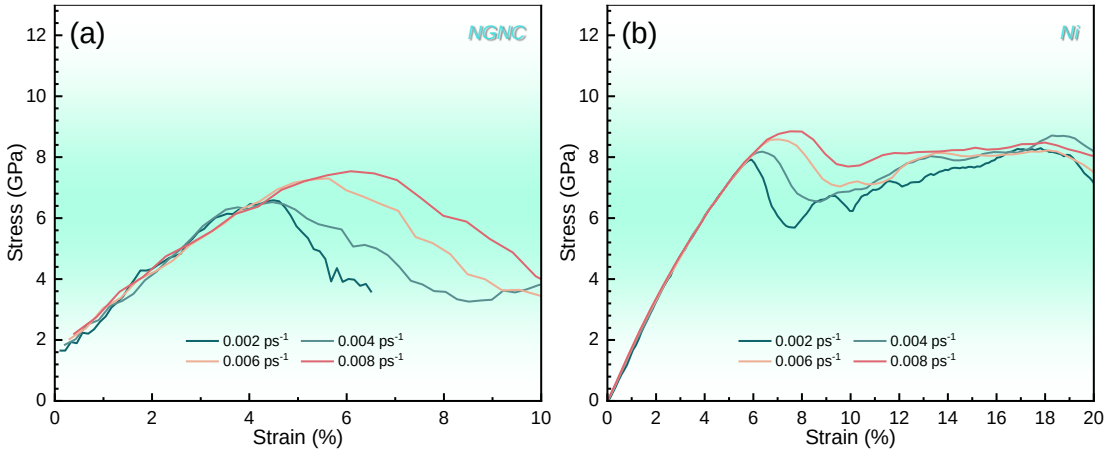

Figure S4. Engineering stress–strain curves measured at 300 K with a PKA energy of 5.0 keV in hydrogen-free environments, comparing different strain rates. (**a**) NGNC. (**b**) Single-crystal nickel.

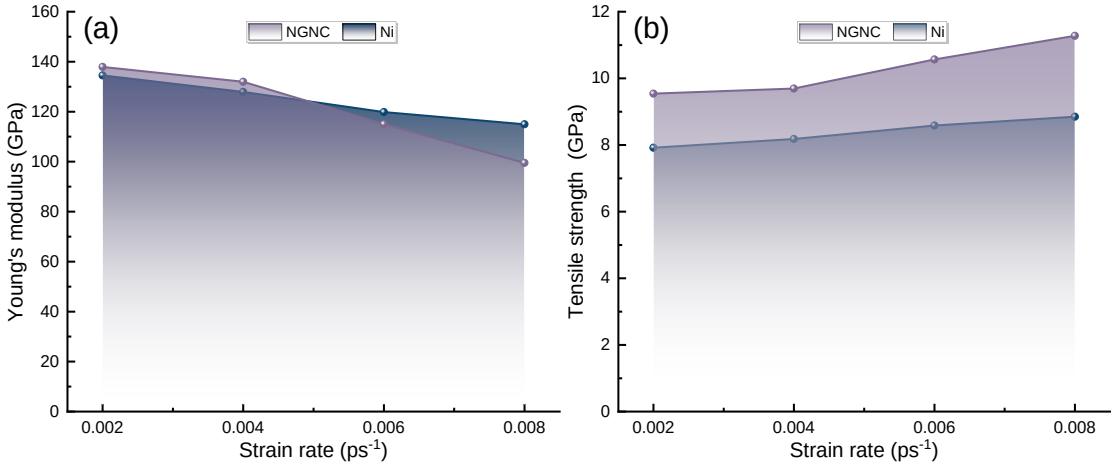

Figure S5. Strain rate dependence of mechanical parameters for NGNC and single-crystal nickel, measured at 300 K with a PKA energy of 5.0 keV in hydrogen-free environments. (**a**)Young's modulus. (**b**) Ultimate tensile strength.

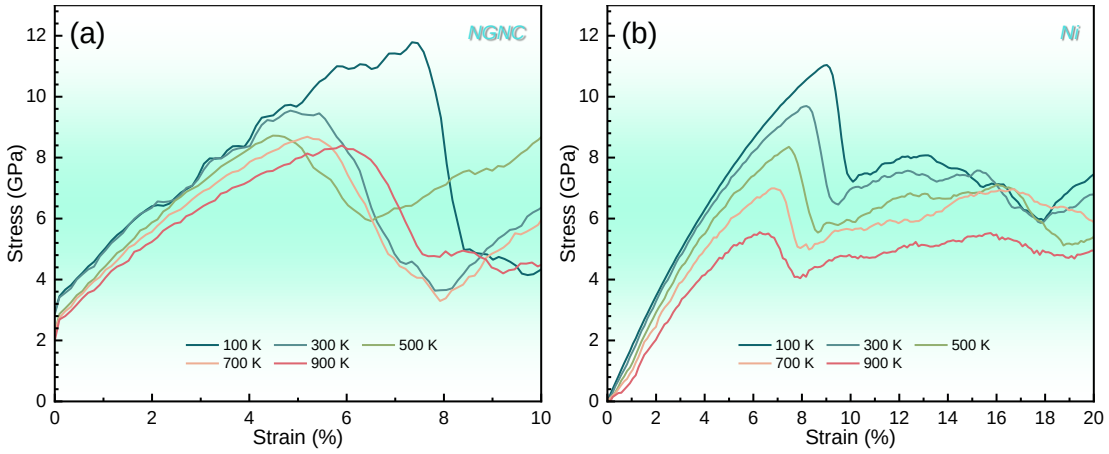

Figure S6. Engineering stress–strain curves measured at a strain rate of 2×10^{-3} ps^{-1} with a PKA energy of 5.0 keV in hydrogen-free environments, comparing different simulation temperatures. (**a**) NGNC. (**b**) Single-crystal nickel.

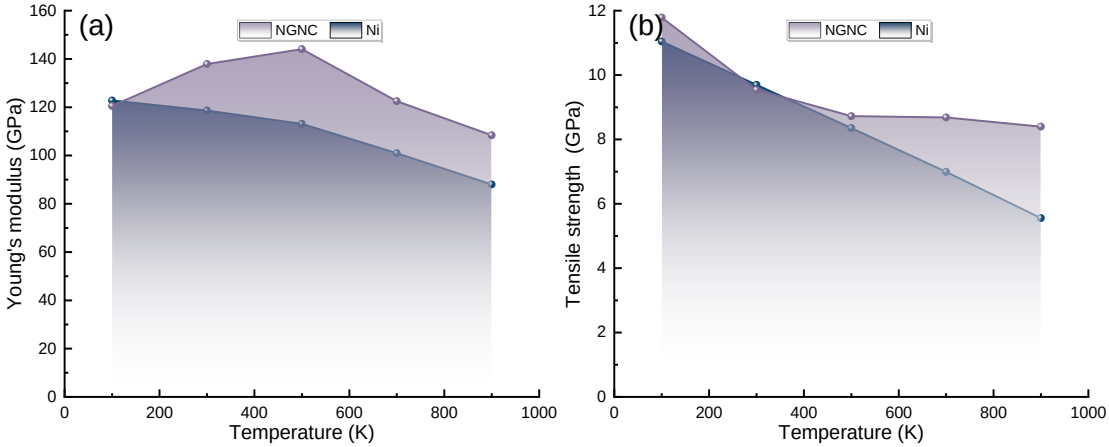

Figure. S7. Simulation temperature dependence of mechanical parameters for NGNC and single-crystal nickel, measured at a strain rate of 2×10^{-3} ps^{-1} with a PKA energy of 5.0 keV in hydrogen-free environments. (**a**)Young's modulus. (**b**) Ultimate tensile strength.