In-plane strain effect on interface stress in Cu/W nano-multilayers

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INTRODUCTION

- The copper/tungsten (Cu/W) system combines the good electrical and thermal properties of Cu with the excellent mechanical properties of W.
- Due to complete immiscibility and incompatibility between Cu and W, interface effects play an important role in Cu/W multilayers and the resulting material properties can be tailored for industrial applications through microstructural and interfacial design.
- Interface stress is one of the fundamental thermodynamics parameters related to interface boundaries in strict relation to interface energy.
- Interface stress is the variation of interface energy with the applied in-plane strain, i.e., interface stress is the work needed to deform the pre-existing interface area elastically, thus providing information about the stability and equilibration of boundaries.

OBJECTIVES

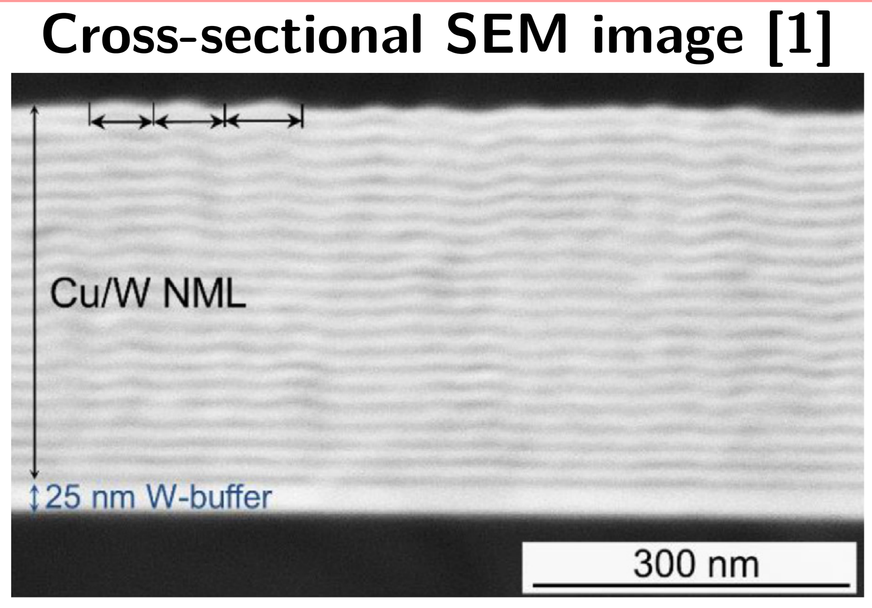
- Combination of experimental observations and modeling approaches to investigate the relationship between in-plain strain and interface stress, using Cu / W nano-multilayers as a model system.

EXPERIMENTAL DETAILS

Cu/W nano-multilayers:

- are produced by DC magnetron sputtering
- composed of alternating 10 nm Cu and 10 nm W layers
- demonstrate Cu{111}/W{110} out-of-plane orientation relation
- develop different in-plain strain depending on Ar pressure

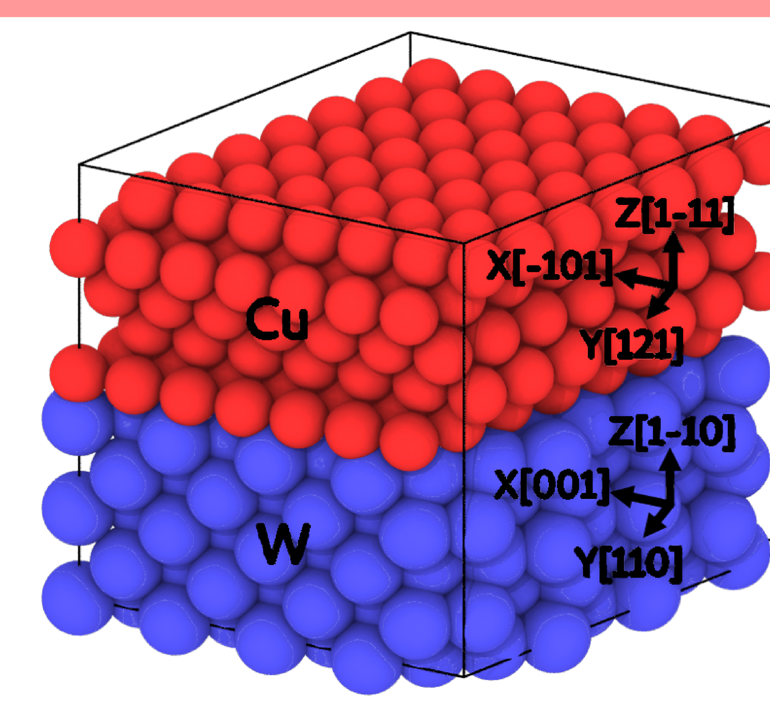
Cross-sectional SEM image [1]



AB INITIO CALCULATIONS

Density functional theory (DFT) calculations are done using:

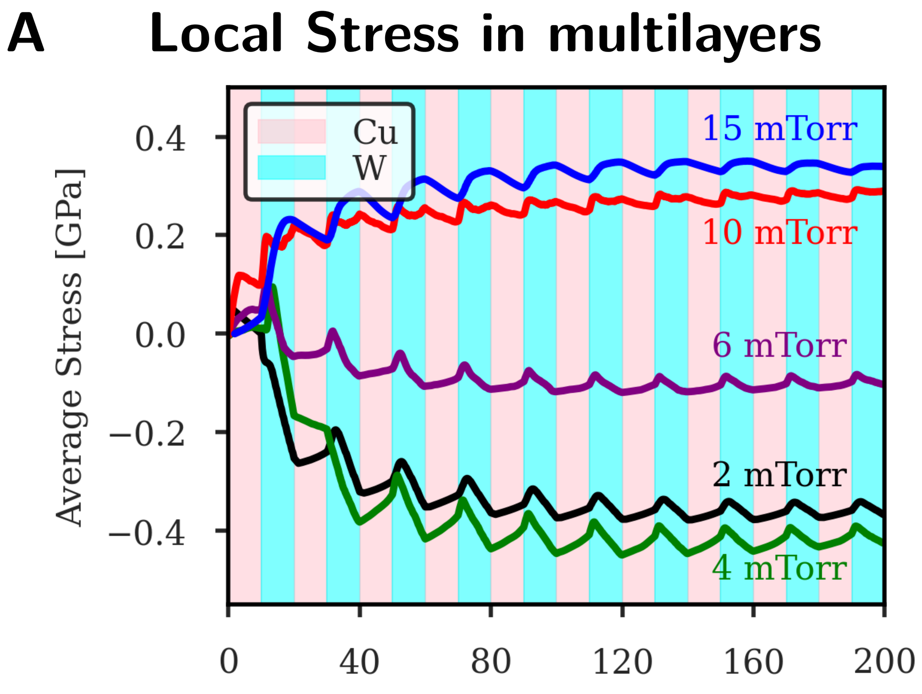
- the bilayer containing 245 Cu atoms and 200 W atoms generated via the CellMatch code [2].
- the CP2K code [3].
- the Goedecker–Teter–Hutter pseudopotential [4]



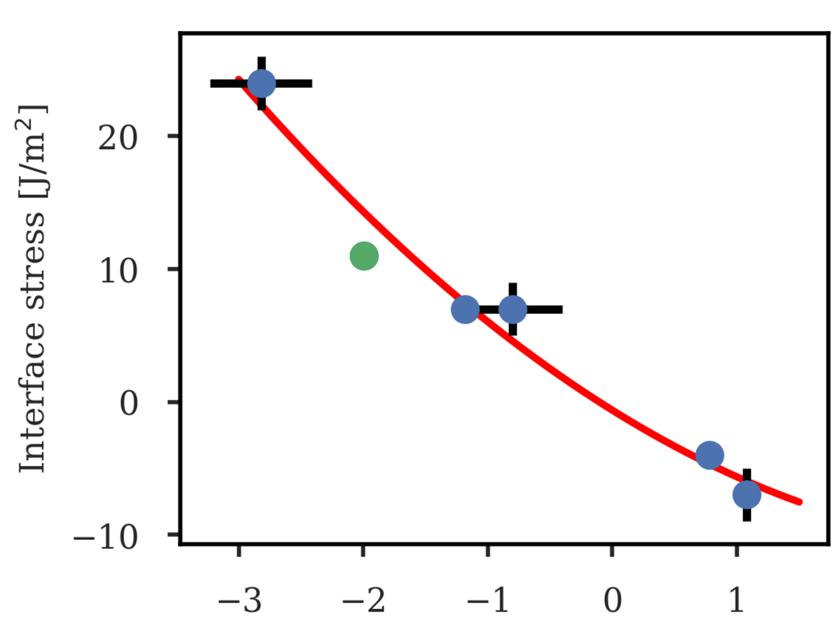
RESULTS

EXPERIMENTS

A Local Stress in multilayers



B Interface Stress



Interface stress, f^ϵ, from interface energy, γ^ϵ, under applied strain ϵ [5]:

$$f^\epsilon = \gamma^\epsilon + \left.\frac{\partial \gamma}{\partial \epsilon}\right|_\epsilon . \quad (1)$$

Interface stress, f^ϵ, from the bilayer in-plane stress, $\sigma^\epsilon_{Cu/W}$:

$$f^\epsilon = -\frac{\lambda^\epsilon}{2}\sigma^\epsilon_{Cu/W}, \quad (2)$$

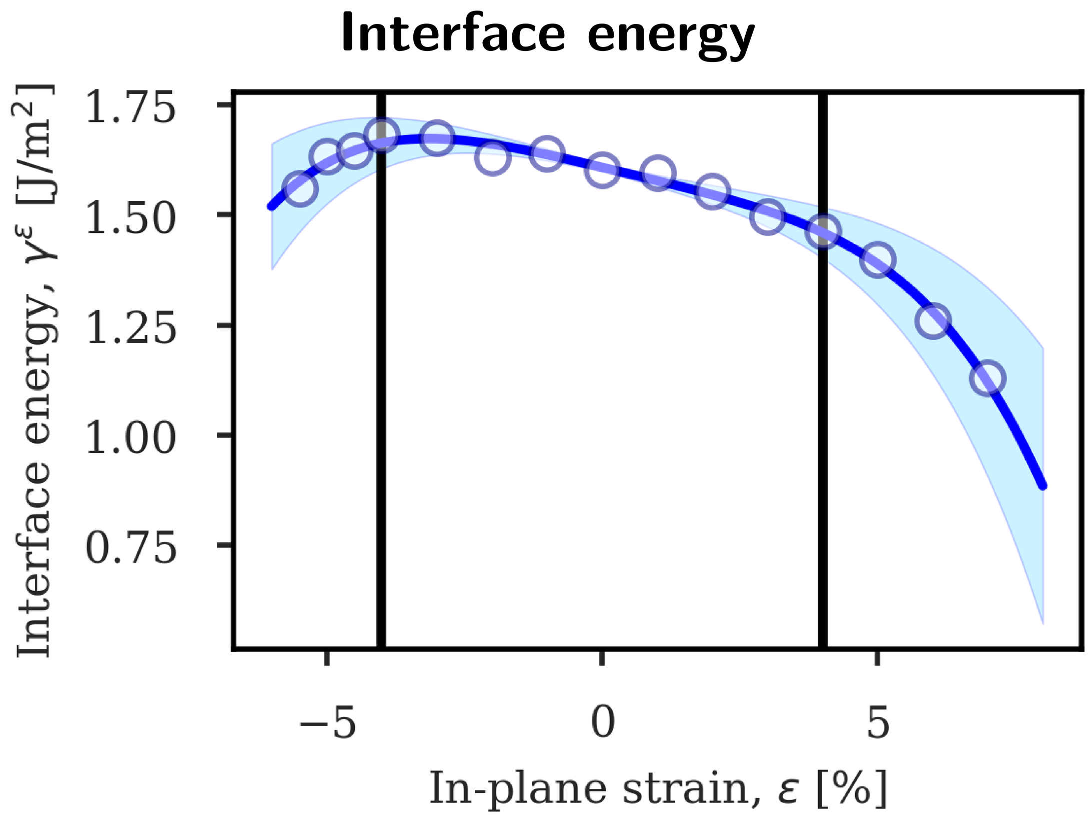
where λ is the bilayer thickness. In experiments, this equation becomes:

$$\sigma_{\mathrm{SC}} - \langle\sigma\rangle_{\mathrm{XRD}} = \frac{2f}{\lambda}, \quad (3)$$

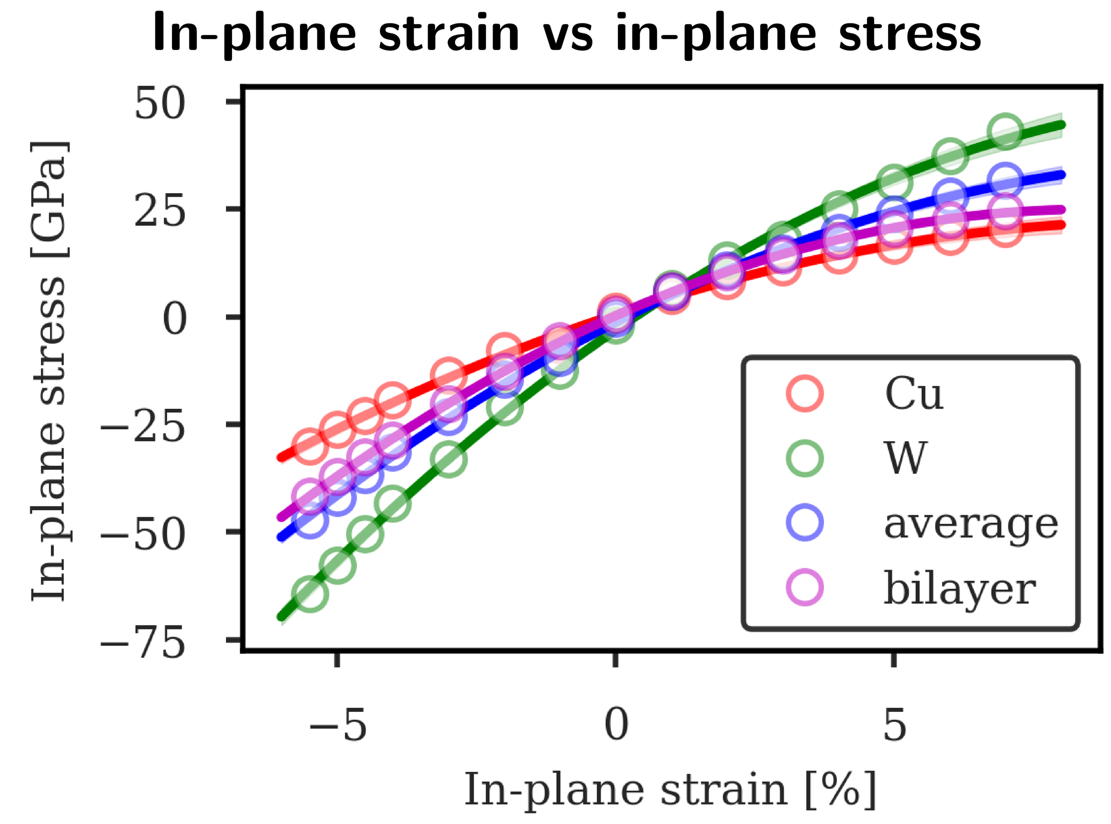
where $\langle\sigma\rangle_{\mathrm{XRD}}$ is the average stress in the Cu and W layers and σ_{SC} is the stress measured from the curvature of the substrate.

AB INITIO CALCULATIONS

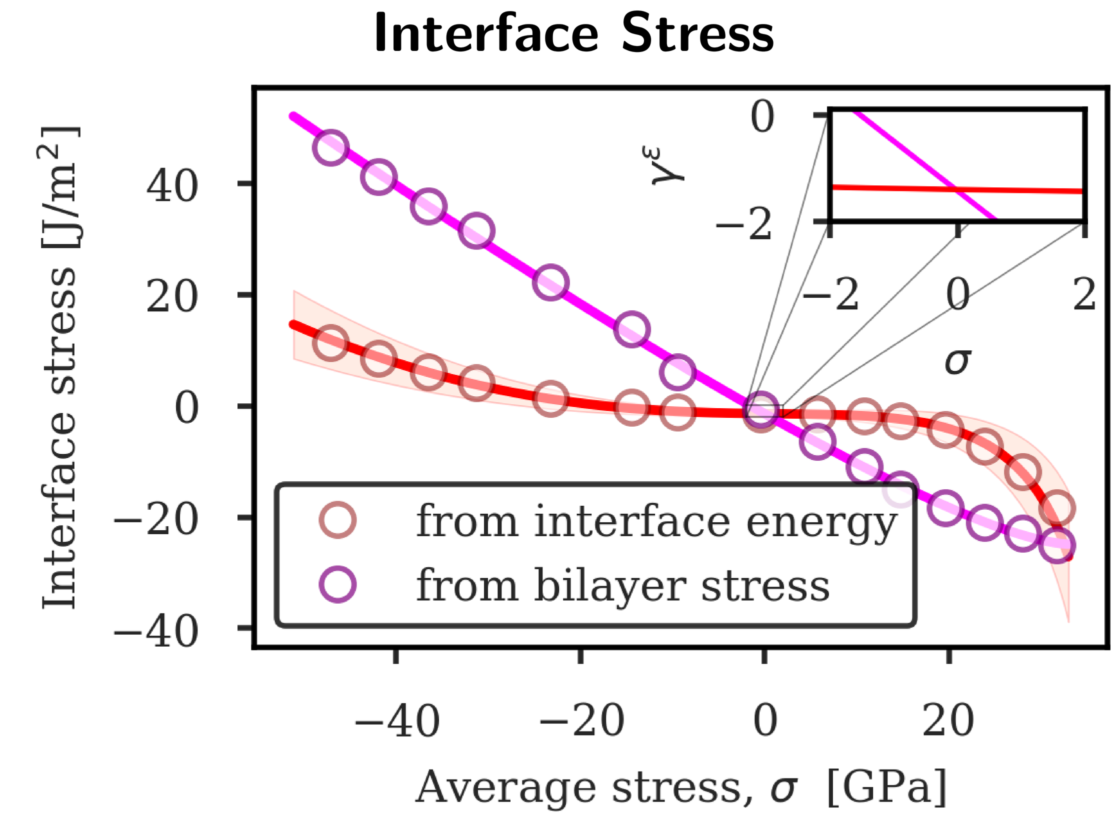
C Interface energy



D In-plane strain vs in-plane stress



E Interface Stress



CONCLUSIONS

- The Cu/W interface stress can be tuned non-linearly from positive to negative by changing the Ar pressure during the deposition of nanomultilayers.
- From DFT calculations, we observe that the change of the interface energy with increasing applied stress is associated with the sharp movement of Cu atoms at the interface and changes in interplanar distances.
- Both derivations of the interface stress only match near zero in-plane strain/average stress, which indicates that Eqs. 2-3 need to be revised to account for high in-plane strain.

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