

# Experimental and computational study of heteroepitaxial thin Fe/Pt spintronic bilayers

Dimitrios Karfaridis<sup>1,\*</sup>, Evangelos Th. Papaioannou<sup>2,3</sup>, Thomas Kehagias<sup>1</sup>, Stefanos Giaremias<sup>1</sup>, Joseph Kioseoglou<sup>1</sup>, George Vourlias<sup>1</sup>

<sup>1</sup>Physics Department, Aristotle University of Thessaloniki, GR 54124 Thessaloniki, Greece

<sup>2</sup>Department of Physics and State Research Center OPTIMAS, Technical University of Kaiserslautern, 67663 Kaiserslautern, Germany

<sup>3</sup>Institute of Physics, Martin-Luther University Halle-Wittenberg, 06120 Halle, Germany

## Introduction & Methodology

In the specific study, Fe (12 nm)/Pt (6 nm) thin bilayers were epitaxially grown by the electron beam evaporation method in ultra-high vacuum conditions, using different substrate temperatures of 30°C, 150°C, 300°C, and 450°C. The epitaxial model was studied by Molecular Dynamics with Monte Carlo simulations. The simulations were experimentally confirmed by X-ray photoelectron spectroscopy. The magnetic anisotropy and static magnetic properties of the different samples were compared by magneto-optical Kerr effect microscopy in the longitudinal alignment (L-MOKE)

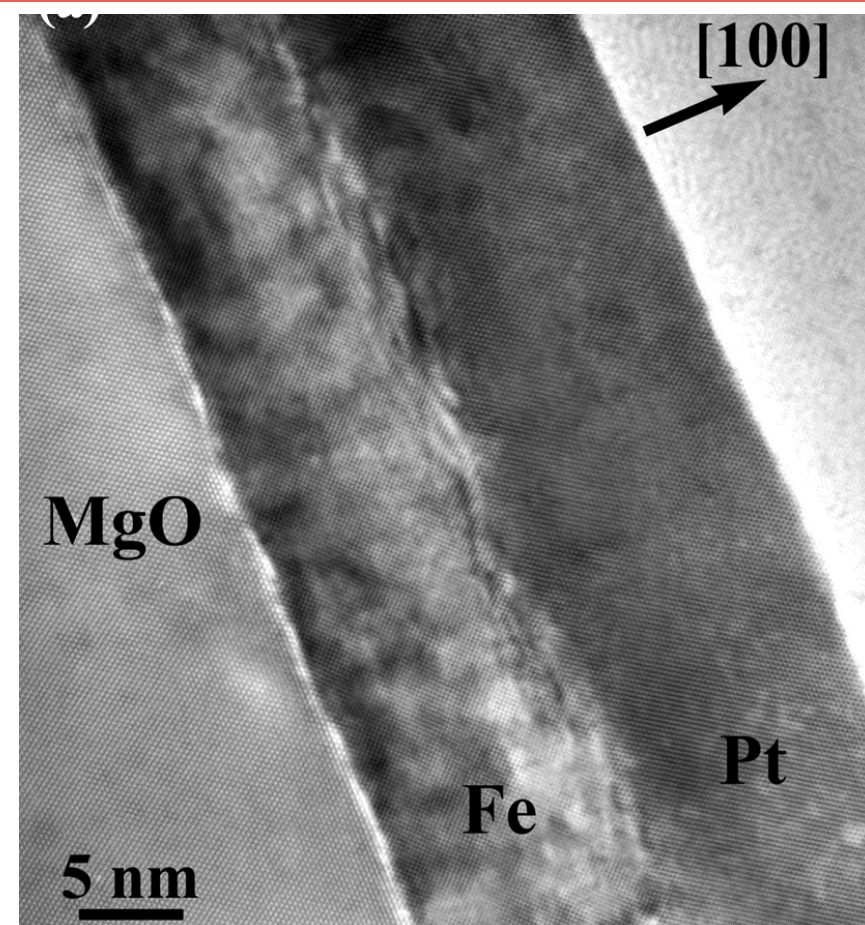


Figure 1: Cross-sectional HRTEM image of the Fe/Pt bilayer deposited on MgO(100). View along the [011]MgO zone axis.

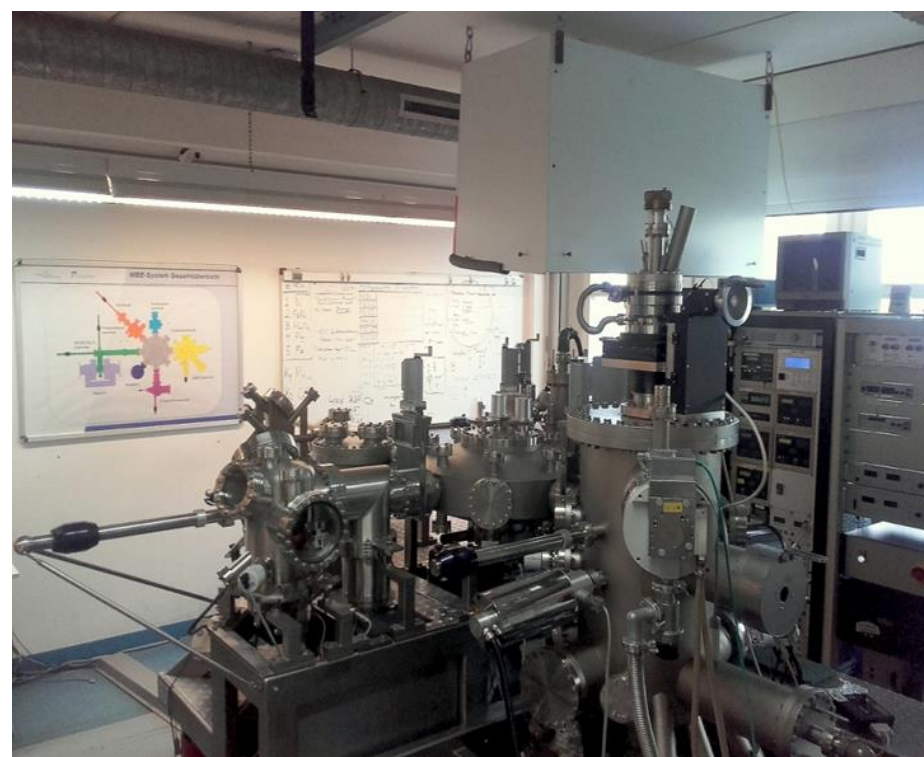


Figure 2: MBE system housed in T.U. Kaiserslautern



Figure 3: Kratos AXIS Ultra DLD XPS and AES spectrometer housed in physics department AUTH.

## Molecular Dynamics simulations

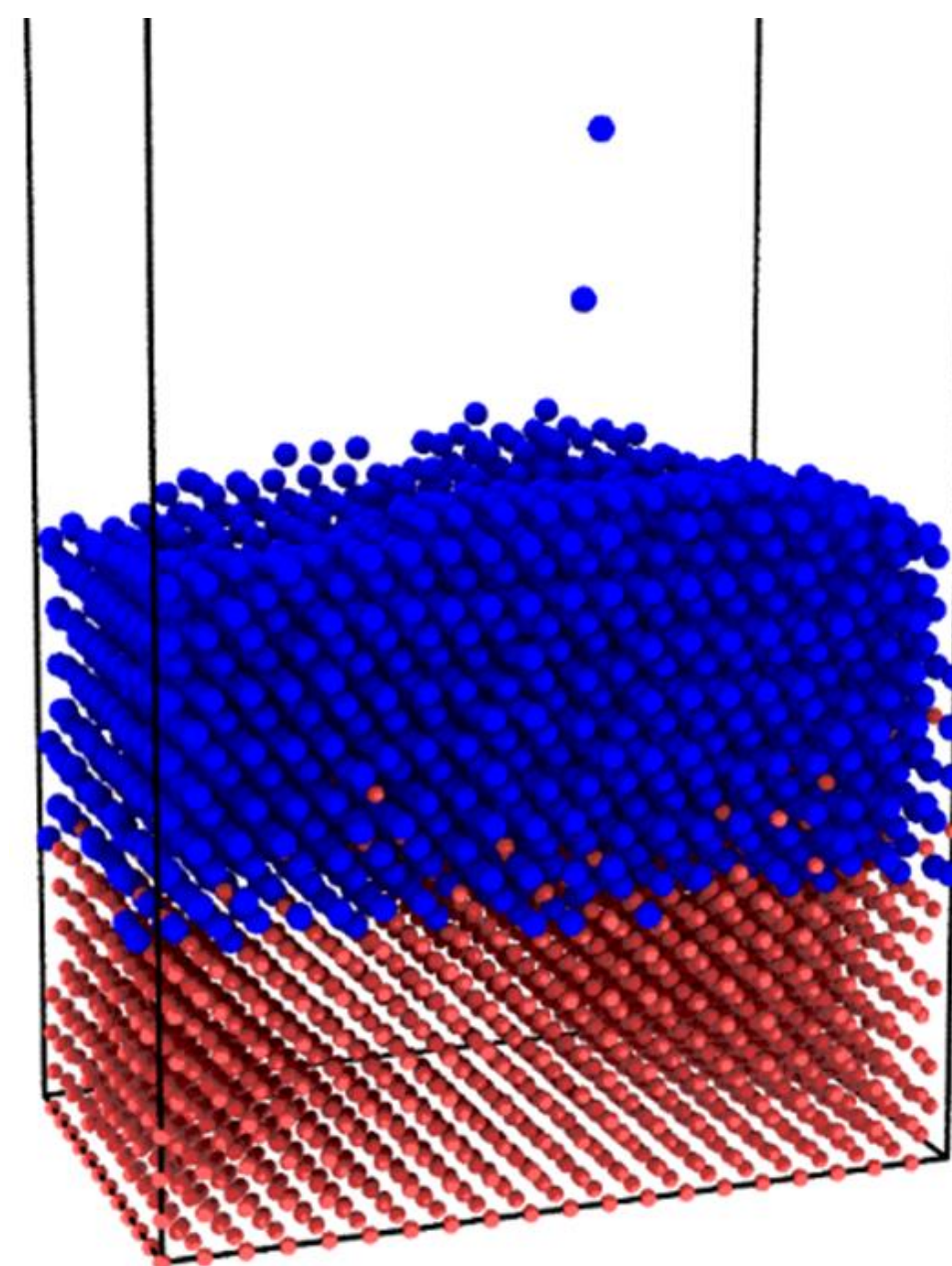


Figure 4: Snapshot during the MD simulated growth, representing the deposition of Pt atoms (blue spheres) on the Fe layer (red spheres). In the process, the weakly bonded Fe surface atoms acquire kinetic energy that causes some of them to diffuse into the growing top layer.

- Pt atoms with *fcc* symmetry
- Pt atoms with *bcc* symmetry
- Fe atoms with *bcc* symmetry

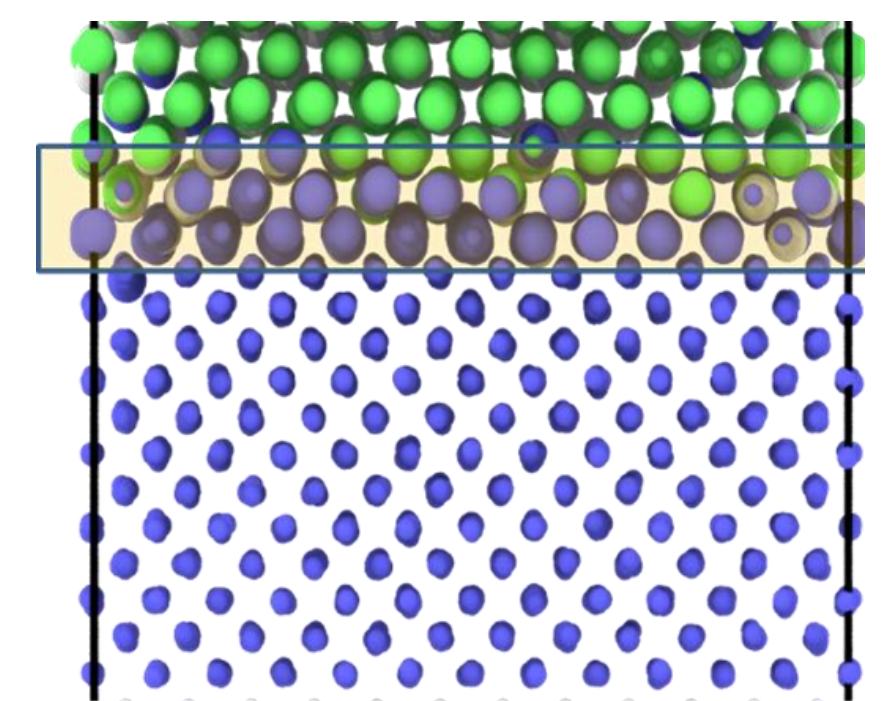


Figure 5: MD Simulations of the lattice symmetry of the two types of atoms during the heteroepitaxy. Pigmentation corresponds to the fcc (green) and bcc (blue) structures of the atoms of Fe (small spheres) and Pt (larger spheres). The highlighted area includes the interface volume, where the Pt atoms have deformed, transforming from the expected fcc to the bcc symmetry.

## Experimental Study

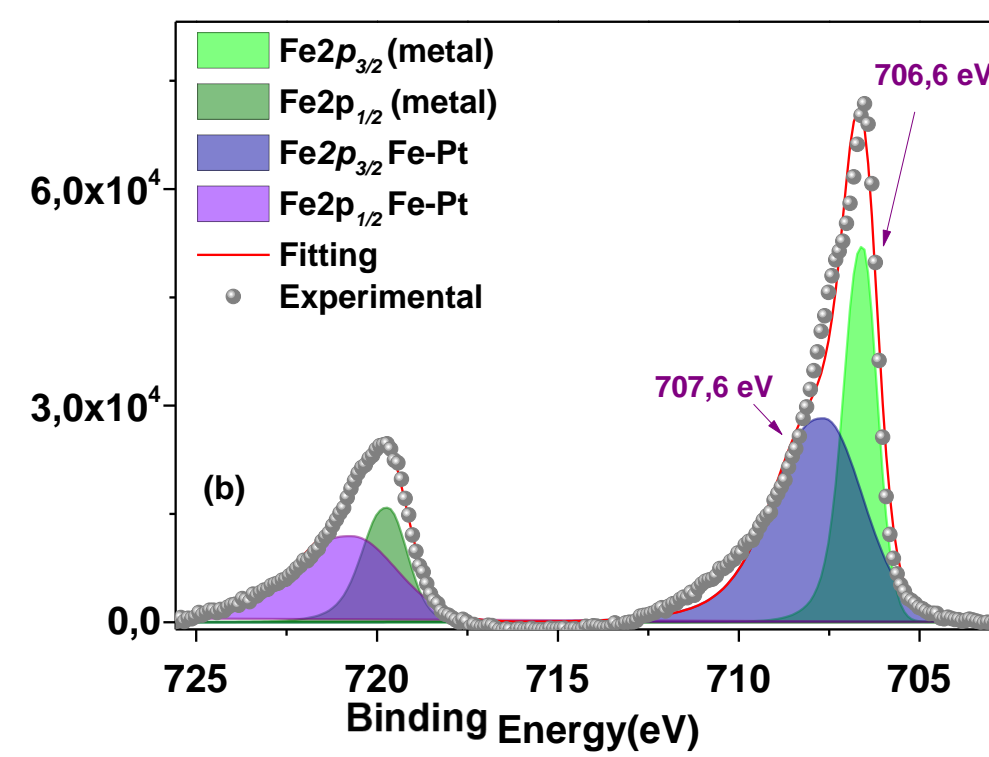
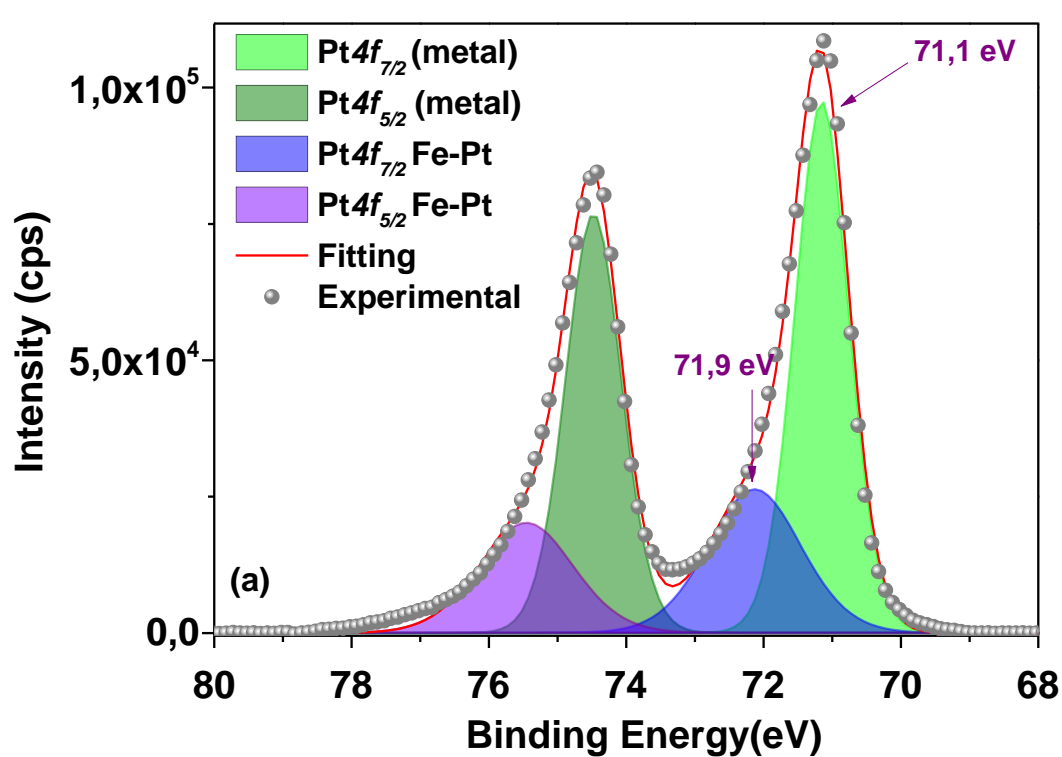


Figure 8: Deconvolution of the XPS experimental HR peaks from the spatial area near the bimetallic interface. (a) The 4f orbitals of Pt for a depth of analysis of 5 nm from the surface. (b) The 2p orbitals of Fe for the same depth of analysis. XPS confirmed the eFe-Pt atomic interactions near the interface.

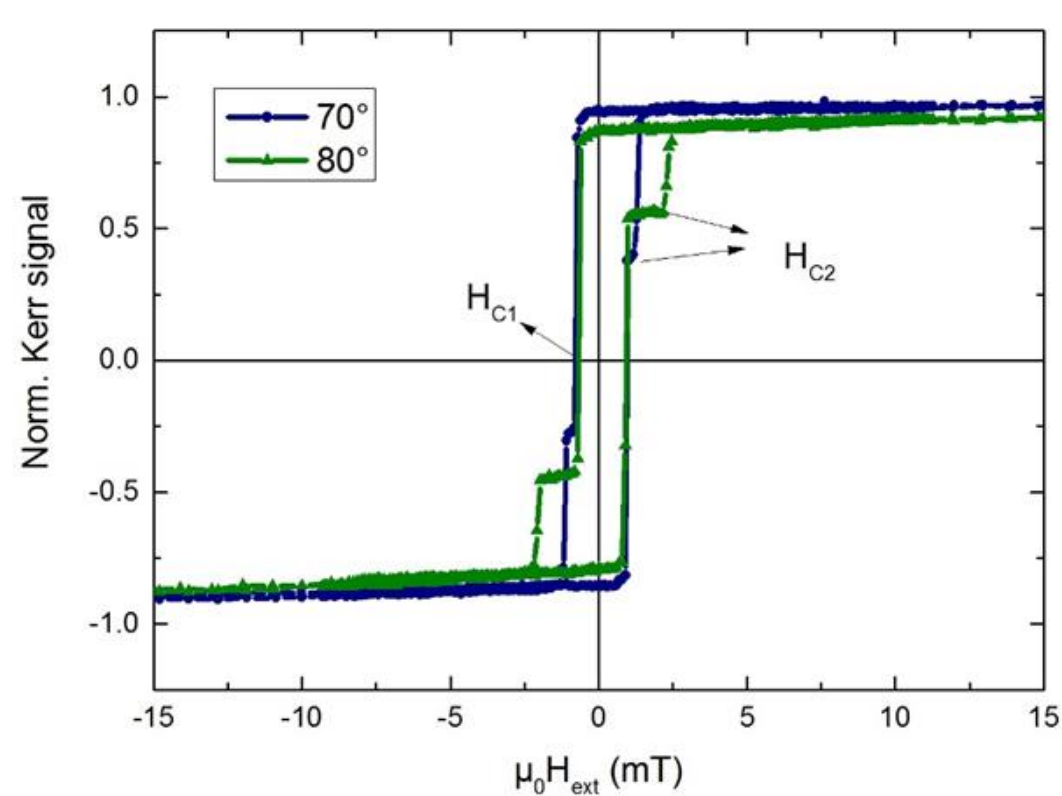


Figure 9: Characteristic hysteresis loops recorded with the help of magneto-optic Kerr effect, at an angle between the external magnetic field and the edge of the sample of  $\theta = 70$  and  $80$  degrees.

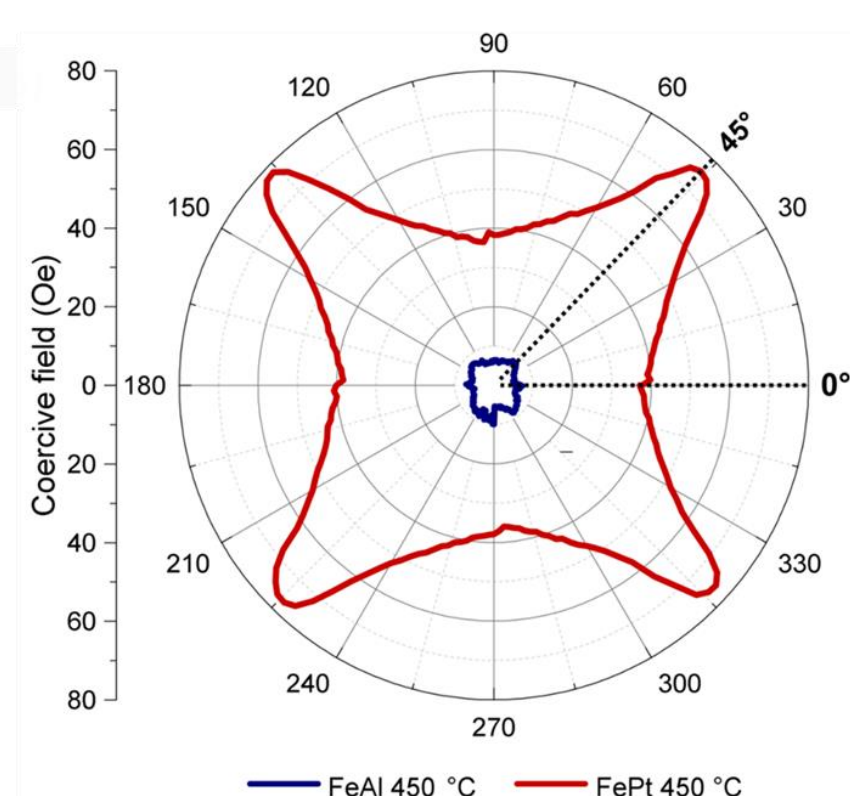


Figure 10: Angular resolved L-MOKE reveals fourfold anisotropy and a strong increase in magnetization for samples with the increase of the growth temperature. Here Fe/Pt at 450°C

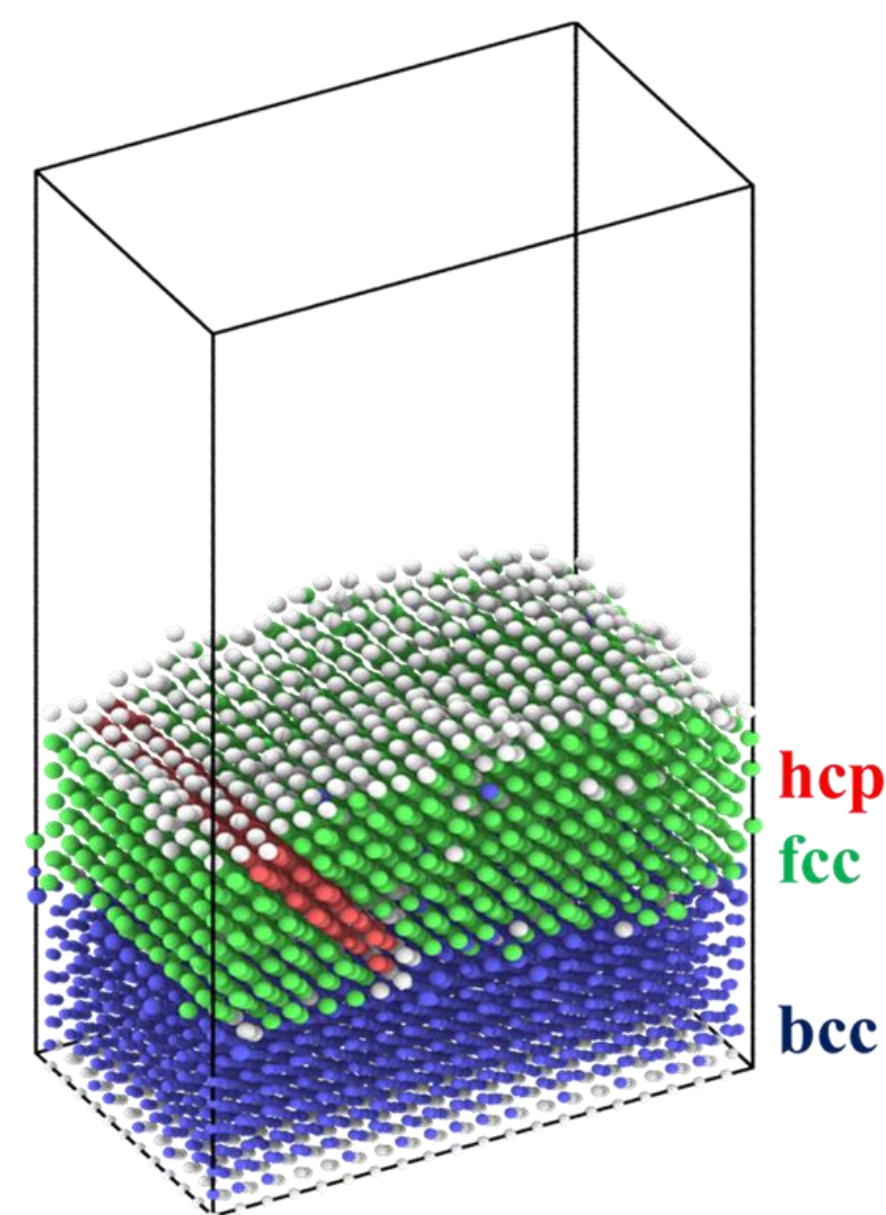


Figure 6: The resulting structural configuration of MD for the Fe/Pt bilayers system. The color coding represents the results of CNA. In particular, the blue atoms represent the structure of Fe receiving the bcc crystal symmetry, the green atoms represent the typical fcc structure of Pt, and the red atoms represent Pt atoms with the hcp lattice symmetry, forming intrinsic stacking faults or incoherent twin boundaries.

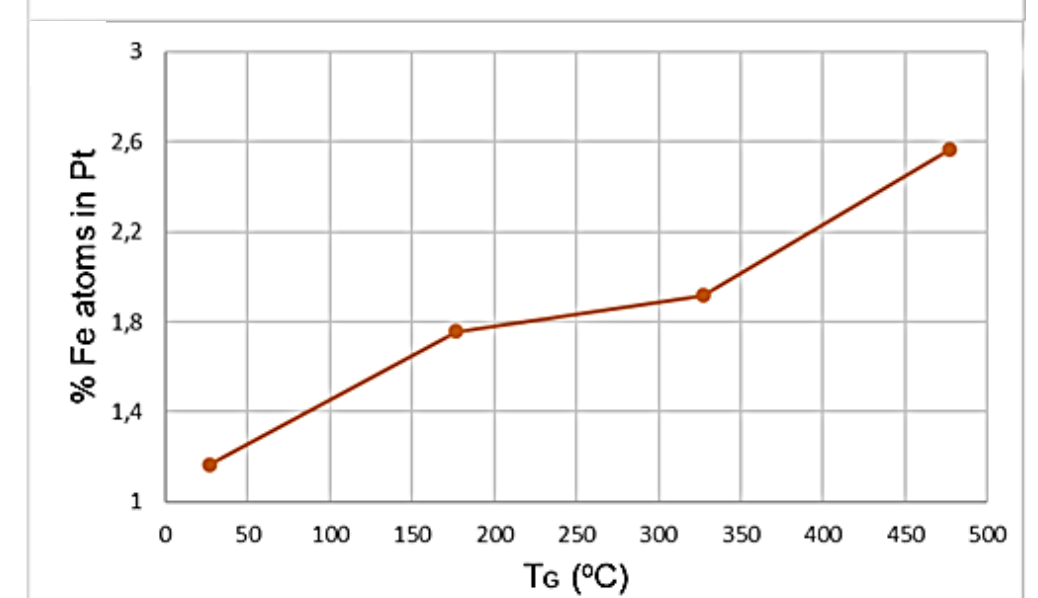
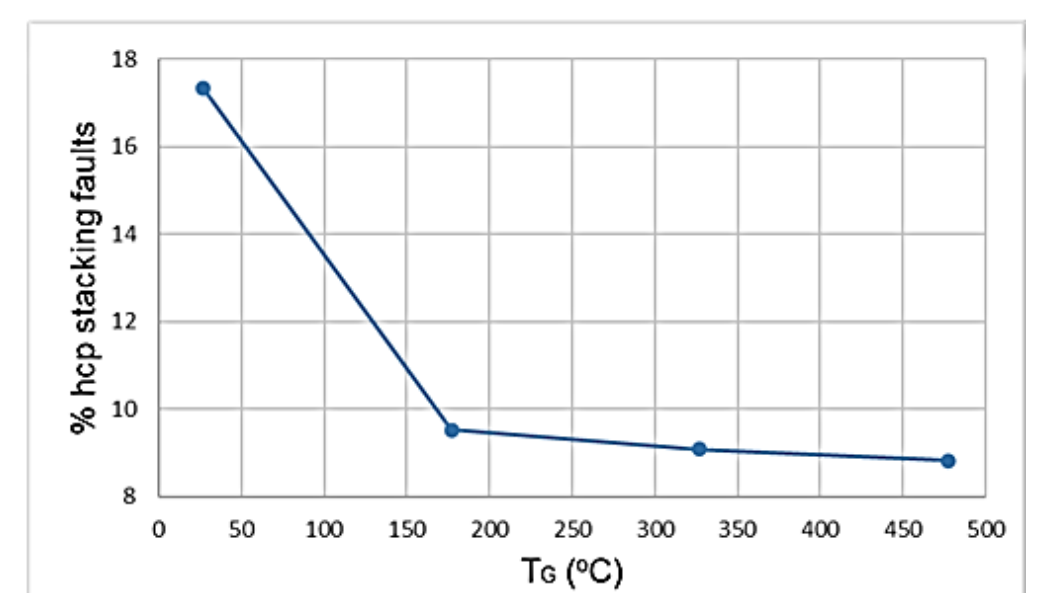


Figure 7: Percentage of hcp coordinated atoms within the Pt layer as a function of the deposition temperature.

## References

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