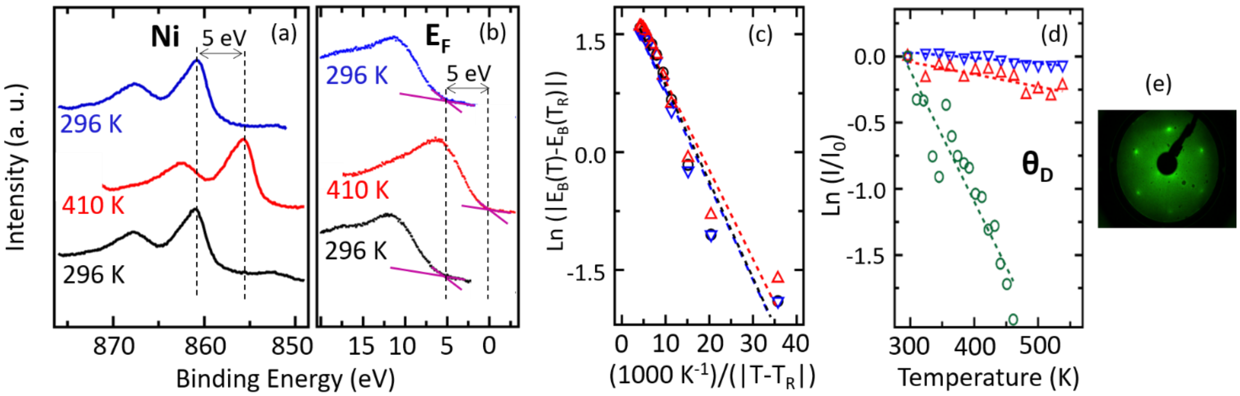

Fig. 1. The XPS spectra of the (a) Ni $2p_{3/2}$ core level and (b) Fermi level (E_F) edge of $NiFe_2O_4$ thin film at 296 K (black spectra) before annealing, at 410 K (red spectra) during annealing, and at 296 K (blue spectra) during cooling. (c) Plotted are the linear fits for a modified Arrhenius-type model to the Ni $2p_{3/2}$ (blue inverted triangles), Fe $2p_{3/2}$ (red upright triangles), and O 1s (black circles) core level binding energies (E_B (T)) as a function of temperature. T_R indicates room temperature (296 K) for this work. (d) The logarithmic plot of relative intensities with temperature for the effective bulk (using XPS intensities) and the effective surface (using LEED intensities) from which effective Debye temperatures (θ_D) can be extracted. The blue inverted triangles, red upright triangles, and green circles are respectively for Ni $2p_{3/2}$, Fe $2p_{3/2}$, and LEED relative intensities. (e) LEED image of $NiFe_2O_4$(111) thin film surface, taken for 133 eV electron energy at room temperature, indicating high surface crystallinity of the thin film.

The main peak positions in XPS spectra represent core level binding energies. In fig. 1a, only Ni $2p_{3/2}$ core level XPS spectra are shown because, for each of the Fe $2p_{3/2}$ and O 1s core level XPS spectra, there exist similar 5 eV core level binding energy shifts between the spectra at room temperature and at 410 K. For clarity, higher temperature spectra at 410 K are shown in fig. 1, but the spectra at other higher temperatures are not shown. In fig. 1d, the slopes of the linear fits give us the effective Debye temperatures. Debye temperature of a given system can be estimated through the Debye−Waller model [1]. Since LEED technique is more surface sensitive technique compared to XPS technique, LEED intensity change with temperature provides us with the estimate for more surface sensitive effective Debye temperature.

Reference:

[1] A. Dhingra, A. Lipatov, M. J. Loes, A. Sinitskii, and P. A. Dowben, ACS Materials Lett. **3**, 414 (2021).