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Supporting information for article:

Temperature evolution of Fe-27Ga structure: comparison of *in situ* X-ray and neutron diffraction studies

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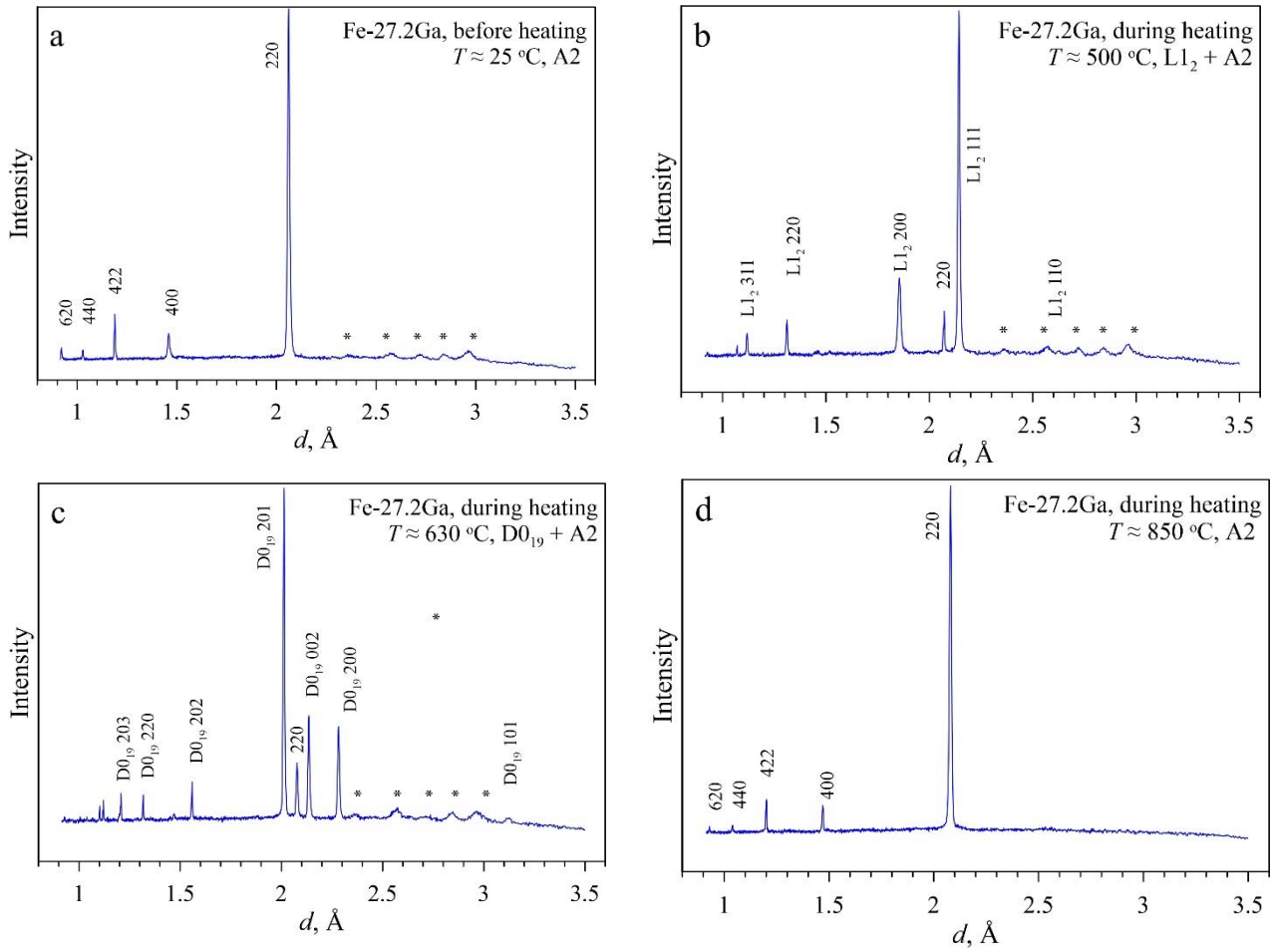

Figure S1 XRD patterns of Fe–27Ga alloy measured at the X-Ray PANalytical Empyrean diffractometer during heating from room temperature to 850 °C. Miller indices and vertical bars indicating the positions of the diffraction peaks are given for the $D0_3$ unit cell. Miller indices for the A2 phase are multiplied by 2 and given as for the $D0_3$ phase. The presence of weak superlattice reflexes which prove the existence of ordered $L1_2$ phase around 500°C and $D0_{19}$ phase around 630°C, respectively are shown in (b) and (c). The diffraction peaks from Ga_2O_3 are marked with asterisks.

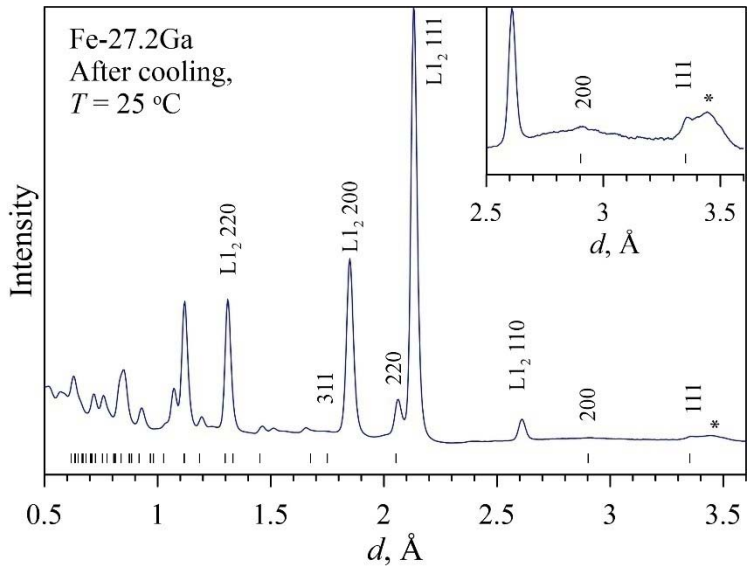

Figure S2 Sum of neutron diffraction patterns of Fe–27Ga alloy measured in the temperature range from 400 °C to room temperature. This pattern proves the presence of low-content $D0_3$ phase but not A2 by the presence of superlattice peaks in diapason from 450 °C to room temperature. The diffraction peak from boron nitride is marked with an asterisk.

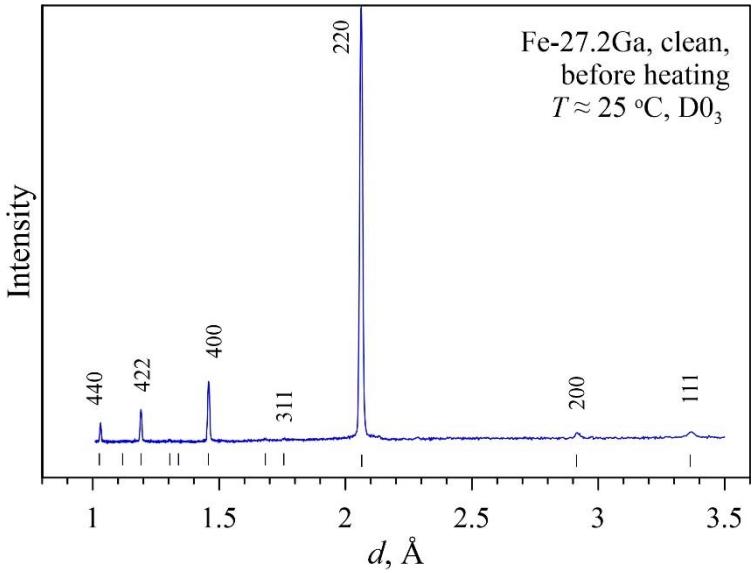

Figure S3 X-Ray diffraction pattern of Fe–27Ga sample subjected to additional polishing after water quenching and before *in situ* heating–cooling measurement.

S1. Debye temperature determination from experimental XRD data

The Debye–Waller factor has a strong impact on high-order diffraction peaks in accordance with Equation 1:

$$D_{hkl} = \exp\left[-\frac{B(T)}{4d_{hkl}^2}\right] \quad (1)$$

where $B(T) \sim T/\theta_D$ at high T, and θ_D is the Debye temperature.

Considering that the measured integrated intensity of the peak at position d_{hkl} is proportional to the Debye–Waller factor:

$$I(d) \sim \exp\left[-\frac{B(T)}{4d_{hkl}^2}\right], \quad (2)$$

for the ratio of the (400) and (422) peaks of the A2 phase, one can write Equation 3:

$$\frac{I_{400}}{I_{422}} \sim \exp\left[-\frac{B(T)}{4a^2}\left((4^2) - (4^2 + 2^2 + 2^2)\right) = \exp\left[\frac{2B(T)}{a^2}\right]\right]. \quad (3)$$

Equation 3 can be transformed as follows:

$$Ln\left(\frac{I_{400}}{I_{422}}\right) = c_1 + c_2 T/\theta_D^2,$$

where c_1 is the constant ratio of structural factors and other contributions in peak intensity and $c_2 = \frac{12h^2}{m \cdot k_B \cdot a^2}$, where h is Plank constant, m the mass of the atom, k_B the Boltzmann constant and a the lattice parameter. Debye temperature is determined from the slope of the plot of $\ln(I_{400}/I_{422})$ versus temperature.

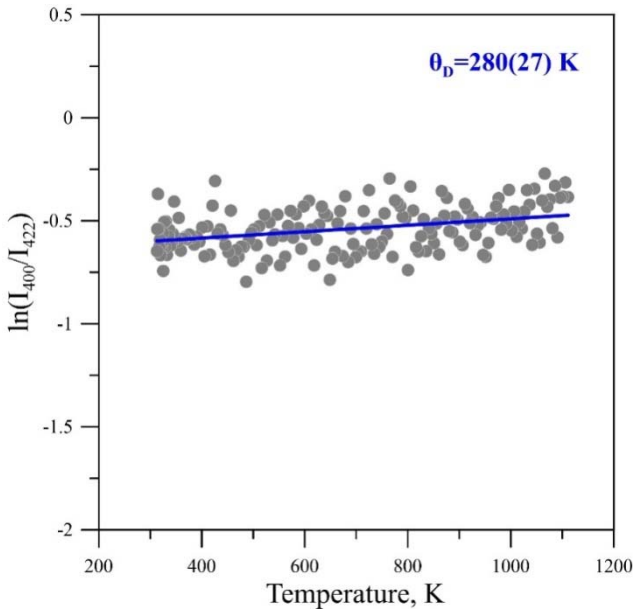

Figure S4 Plot of $\ln(I_{400}/I_{422})$ versus temperature; solid line is a linear fit.