Atomic array reconstruction with giant magnetic response induced by uniaxial stress in MnP

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Uniaxial stress, σ, is one of powerful external fields to achieve anisotropic control of crystal and electronic structures of materials. Recently, we have found that the magnetic susceptibility (// a) in the ferromagnetic phase of MnP is enhanced by the application of σ of 100 MPa // a by a hundred times [1]. This is an irreversible phenomenon and is maintained even after removal of σ. Our previous neutron diffraction experiments using a stress-released sample revealed that this enhancement is caused by the formation of a ``fresh crystalline domain'' in which the original domain is rotated by ±123° along the $b$ axis [1]. This formation of the ``fresh domain'' should be due to the rearrangement of the fractional coordinates of each ion, and therefore, we have named this phenomenon ``an atomic reconstruction''. It remains unknown, however, how much spatial disorder occurs and how long it persists during the process of the atomic reconstruction, because the stress-released sample was used in the previous study.

In this study, we performed a neutron diffraction experiment of MnP under an applied uniaxial stress up to 250 MPa to reveal the *in situ* process and kinetics of the atomic reconstruction. The experiment was conducted using the 4G GPTAS installed at JRR-3 with our homemade uniaxial stress device. To access the (*H*0*L*) plane with the application of σ // a, we designed a horizontal pressure cell.

Figure 1 shows the temperature (T) dependence of the integrated intensity (upper panel) and the FWHM (lower panel) of the 200 reflection. While the integrated intensity is independent of T at the almost ambient condition (20 MPa), it decreases with increasing T until 75 K under applied σ of 120 MPa. This indicates that the volume fraction of the original domain reduces because of the atomic reconstruction by the application of σ. Over 75 K, in contrast, the integrated intensity (σ = 120 MPa) increases with increasing T. We believe that this result is attributable to the change in sample condition from the so-called `extinction affected' to the `extinction free' due to the σ-induced fresh domains. This assumption would be evidenced by the data of 130 MPa, in which the integrated intensity is enhanced by a further increase in σ regardless of some temperature change. On the other hand, the temperature dependence of the FWHM does not show any change even under applied σ. We add that diffuse scatterings are also not observed even under applied σ. These results indicate that on the time scale of the neutron diffraction measurements, each ion ``instantaneously'' belongs to one of the fresh domains and there is no spatial disorder.

We find that a state of the original and fresh domains under applied σ beyond 130 MPa appears different from that stated above, and a comprehensive analysis is underway.

[1] T. Kozawa *et al*., Sci. Rep. **13**, 13750 (2023).

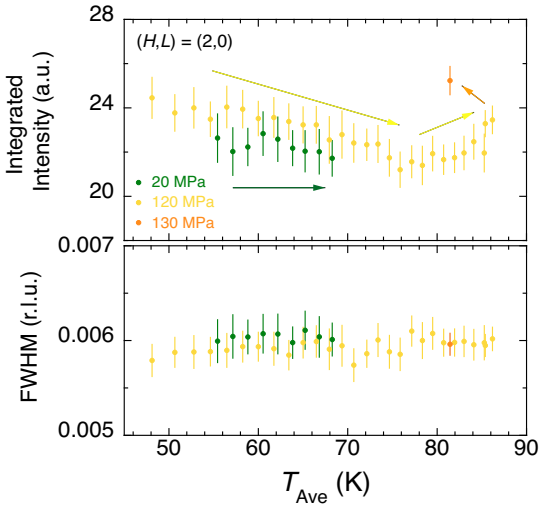

Fig. 1. Temperature dependence of the integrated intensity (upper panel) and the full width at half maximum (FWHM) (lower panel) of the 200 reflection at almost ambient pressure (20 MPa) and under applied stress (120 and 130 MPa).