Magnetic-field driven domain wall evolution in rhombohedral magnetostrictive single crystals: a phase-field simulation

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Supplementary Note 1: The process of domain formation was simulated using the phase-field method, with a dimension of 512Δx × 512Δx × 32Δx (Δx = 2 nm).

The findings indicate that the 3D simulation exhibits similar mechanisms compared to the 2D simulation (**Figure 2**). Consequently, the behavior of the 109° and 71° domain walls in reaction to external magnetic fields can be comprehensively elucidated by the 2D simulation with periodic boundary conditions.

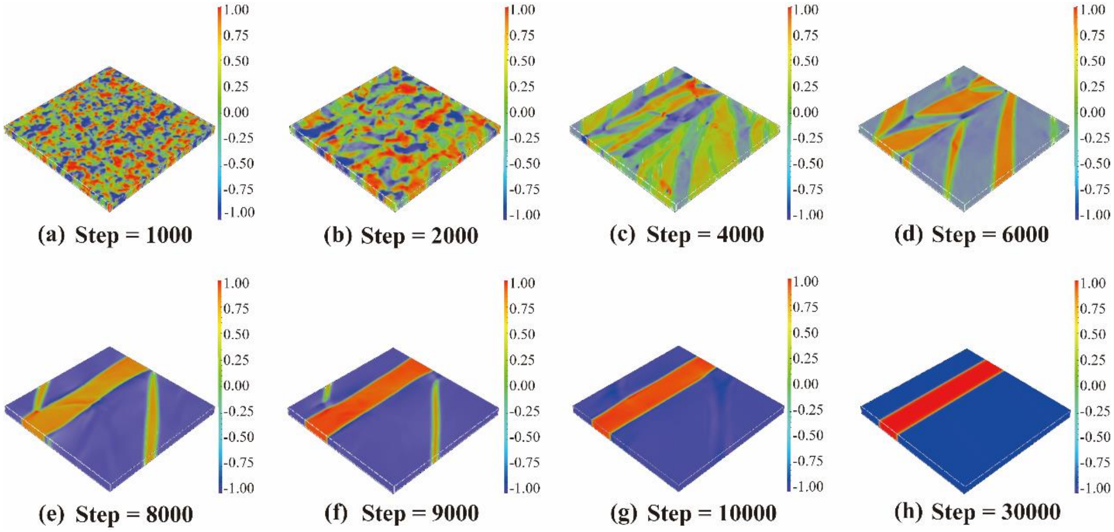

Figure S1. 3D simulation of the domain formation process. The colors represent the magnitude of magnetization along z direction.

Supplementary Note 2: The distribution of stress during the domain formation process of the rhombohedral (Tb-Dy)Fe_2 single crystal in Figure 2.

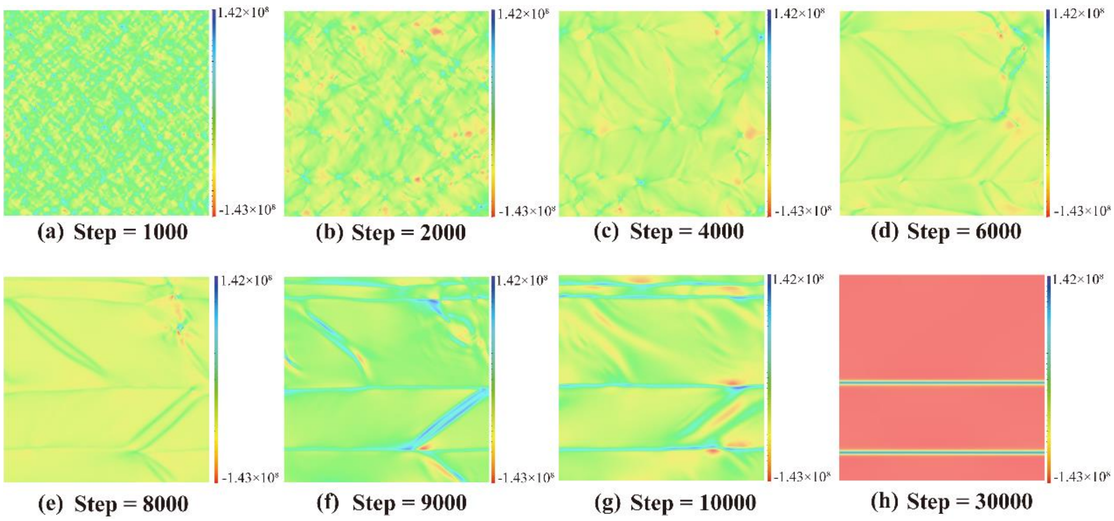

Figure S2. Stress distribution along the z direction during the formation of rhombohedral (Tb-Dy)Fe_2 single crystal domains.

Supplementary Note 3: In the domain configuration exclusively comprising 71° domain wall, the complex magnetization switching is observed in close proximity to the magnetic field's peak, provided that the applied magnetic field surpasses the coercive field.

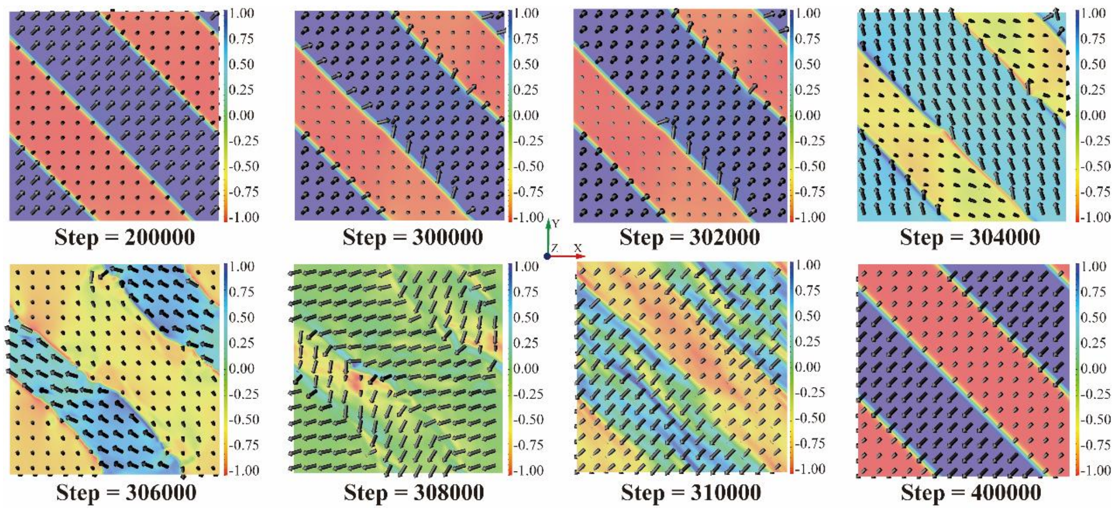

Figure S3. The domain switching in the dashed box near t = T/4 in **Figure 4**. The Step = 200000, Step = 300000, and Step = 400000 are equivalent to t = T/6, t = T/4, t = T/3, respectively.

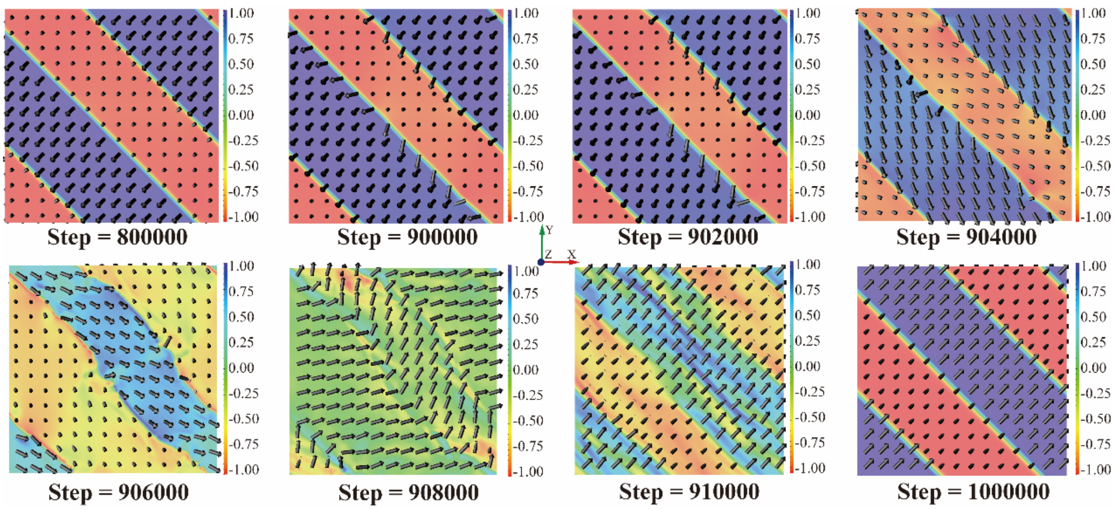

Figure S4. The domain switching in the dashed box near t = 3T/4 in **Figure 4**. The Step = 800000, Step = 900000, and Step = 1000000 are equivalent to t = 2T/3, t = 3T/4, t = 5T/6, respectively.

Supplementary Note 4: In the domain configuration exclusively comprising the 71° domain wall, the magnetostriction of the rhombohedral ferromagnetic single crystals.

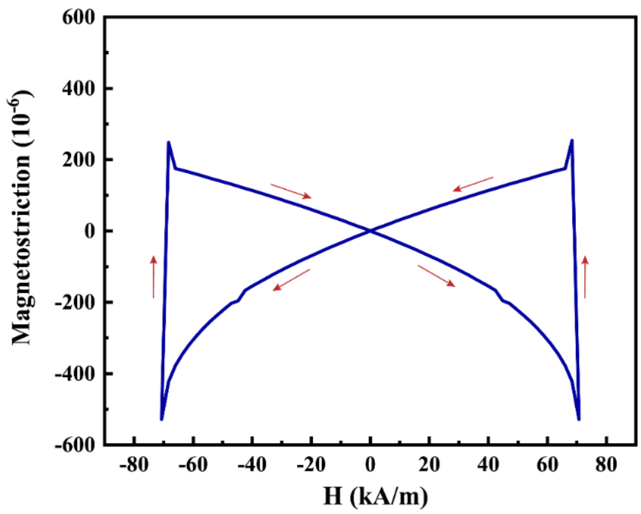

Figure S5. The magnetostriction of the rhombohedral ferromagnetic single crystals in **Figure 4**. Upon reaching the peak values of magnetic fields, the applied magnetic field triggers the complex domain switching, resulting in the magnetostriction 'jump' effect of the rhombohedral single crystal. The red arrows depict the direction of the curve.

Supplementary Note 5: In the domain configuration exclusively comprising the 109° domain wall, the faster movement of the 109° domain walls under the constant magnetic field exceeding 20 kA/m.

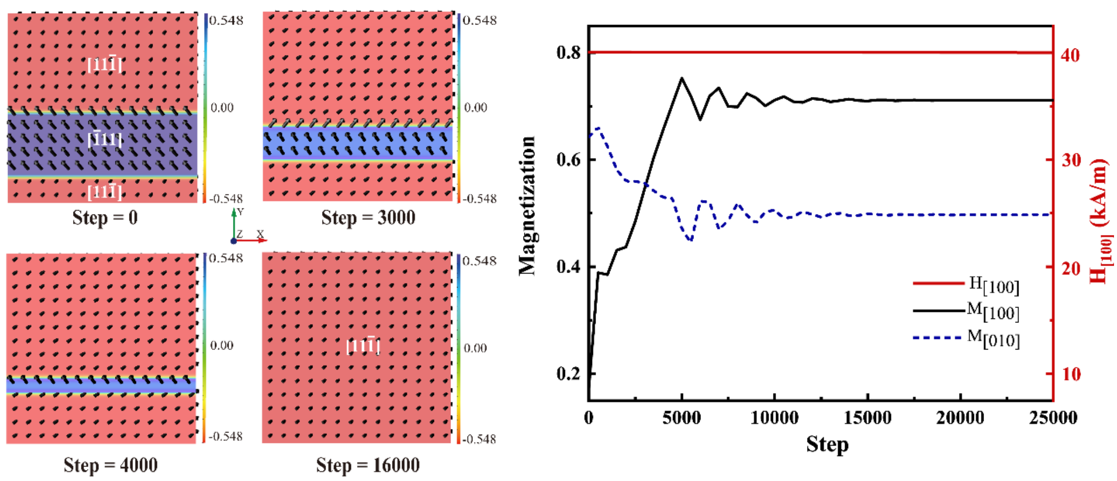

Figure S6. The moving of the 109° domain walls and heterogeneous magnetization switching under the constant magnetic field 40 kA/m.