

Polymorphism and polytypism of α -LiNH₄SO₄ crystals. Monte Carlo modeling based on X-ray diffuse scattering

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Supporting Information

I.

Comparison of calculated
3*kl* section of reciprocal space
and intensity profiles running through 11*l* line
for 1-D model with different interaction parameters *J*
according to the formula

$$H = - \sum_{i=1..n} J \cdot \delta(s_i, s_{i+1})$$

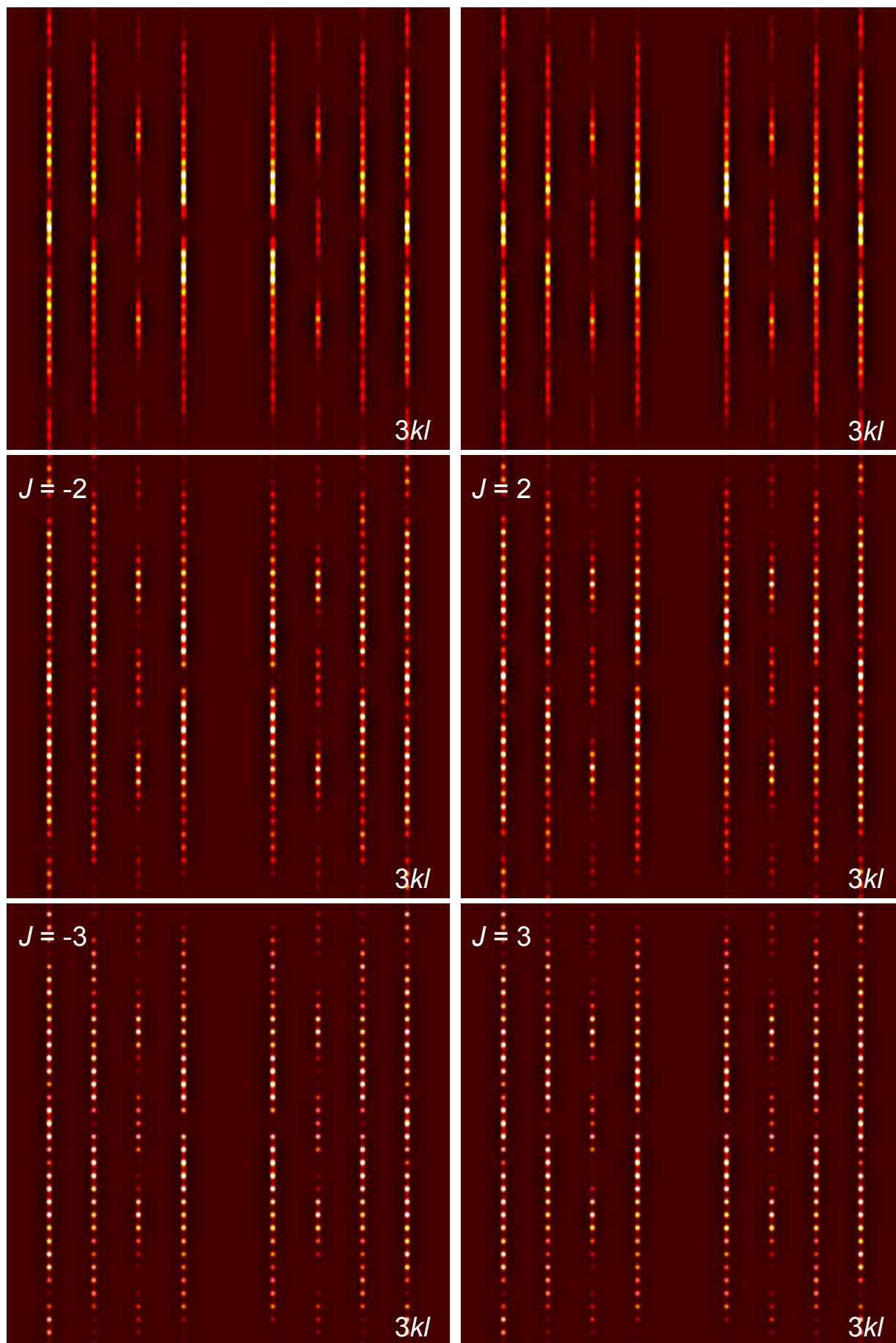


Figure 1. Comparison of calculated $3kl$ section of reciprocal space for 1-D model with different value of interaction parameter $J = -3; -2; -1; 1; 2; 3$.

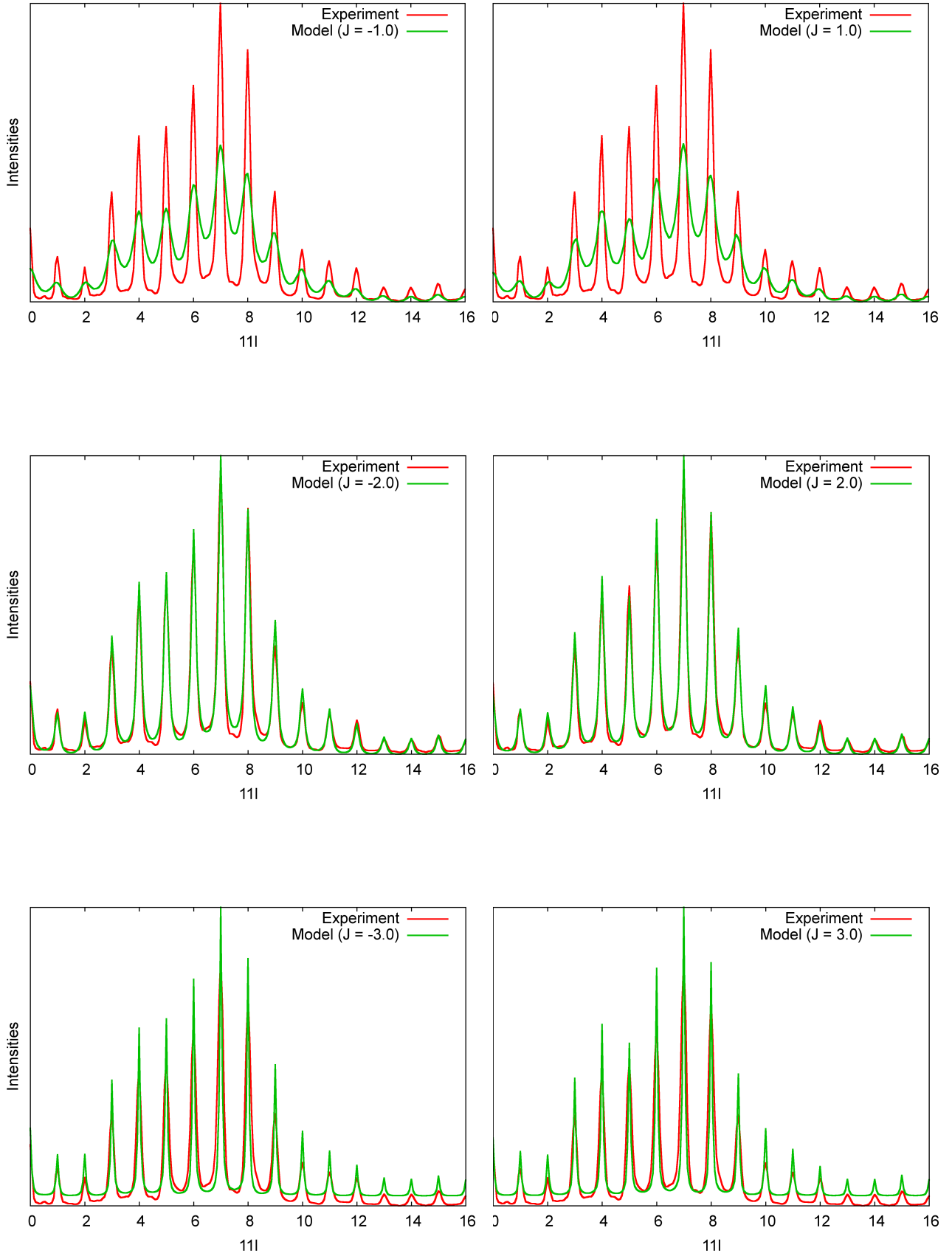


Figure 2. Comparison of calculated intensity profiles running through $11l$ section of the reciprocal space for 1-D model with different value of interaction parameter $J = -3$; -2 ; -1 ; and $J = 1$; 2 ; 3 .

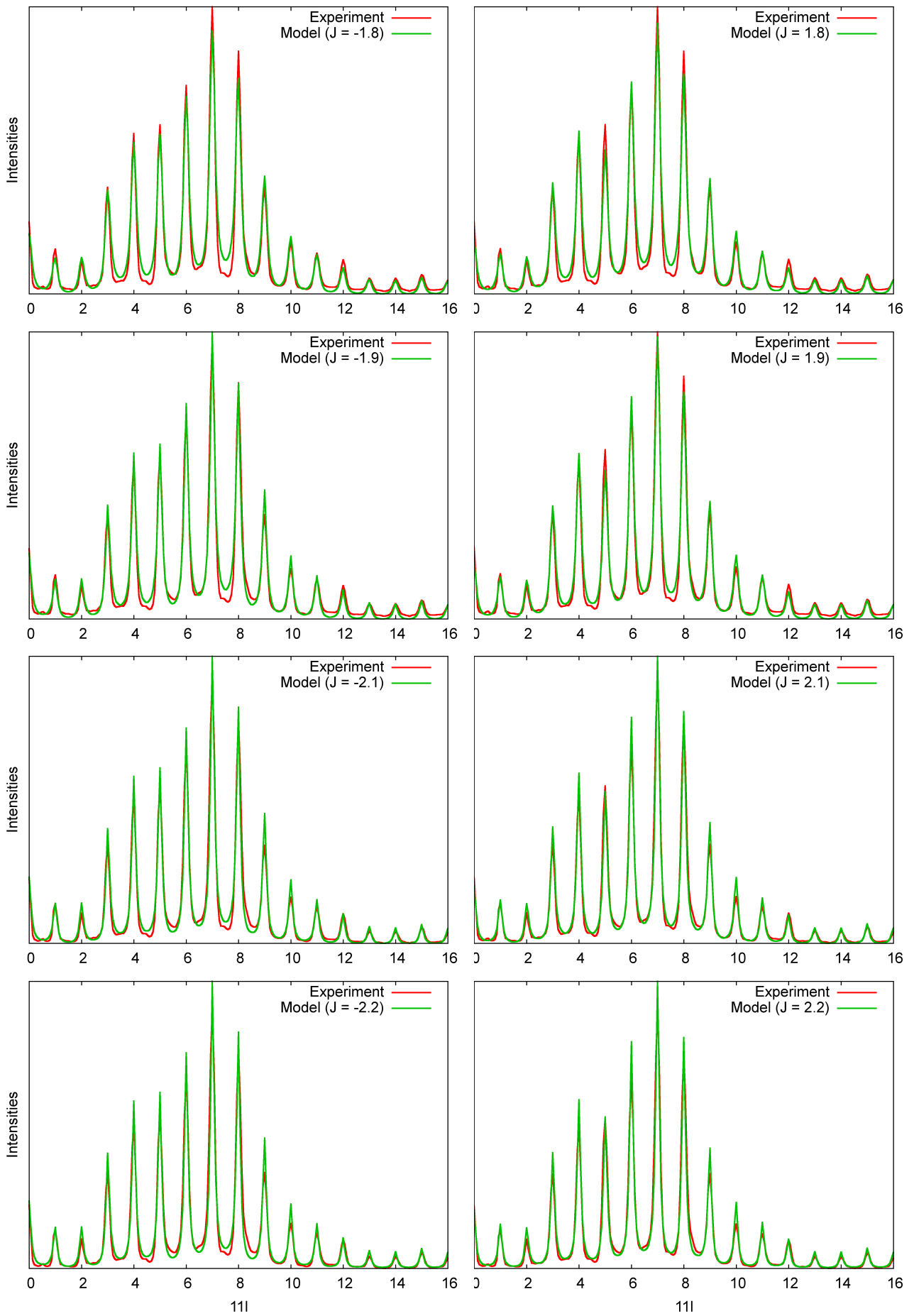


Figure 3. Comparison of calculated intensity profiles running through $11l$ section of the reciprocal space for 1-D model with interaction parameter $J = -1.8; -1.9; -2.1; -2.2$ and $J = 1.8; 1.9; 2.1; 2.2$.

II.

Calculated $h1l$, $h2l$ and $h3l$ sections of reciprocal space for 2-D model with different interaction parameters J_I^a and J_I^c according to the formula

$$H = - \sum_{i=1..m} J_1^a \delta(s_i, s_{i+1}) + \sum_{j=1..n} J_1^c \delta(s_j, s_{j+1})$$

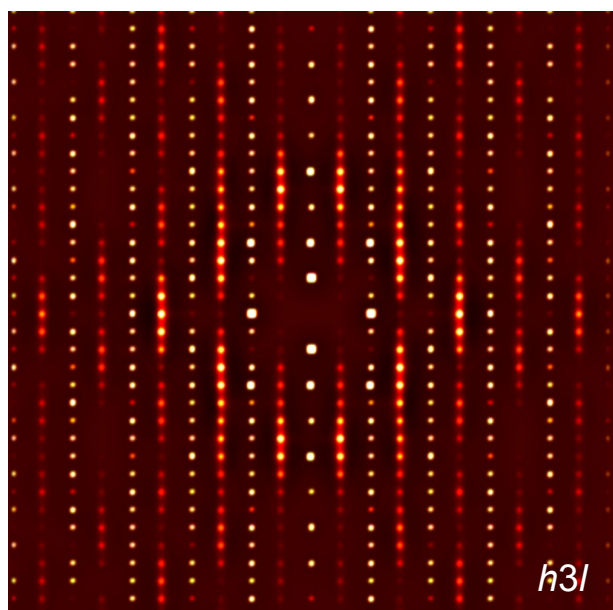
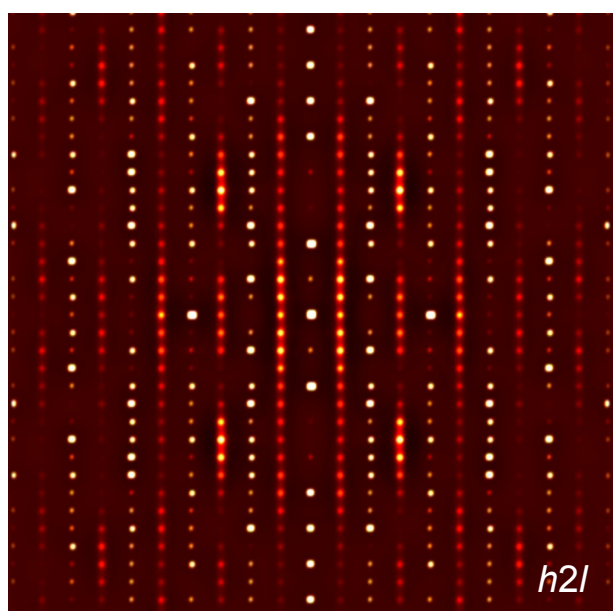
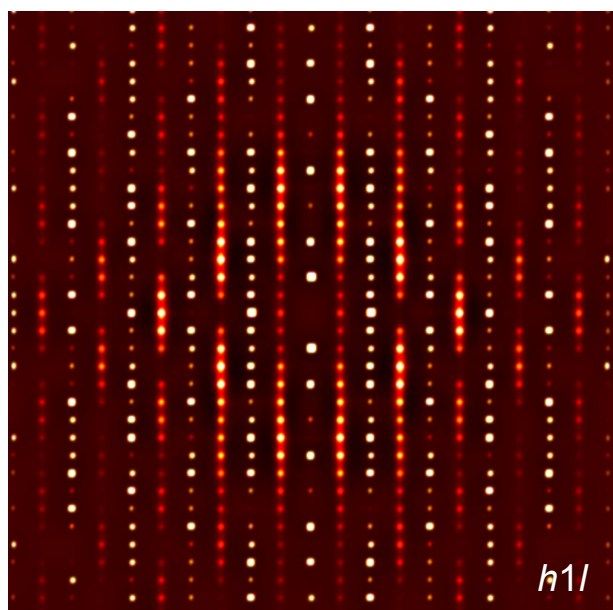


Figure 4. Calculated sections of reciprocal space for 2-D model with interaction parameters $J_I^a = 2$ and $J_I^c = -0.22$.

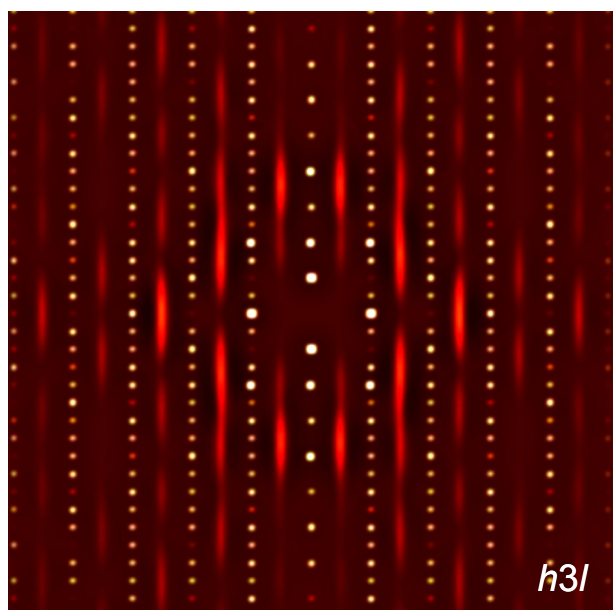
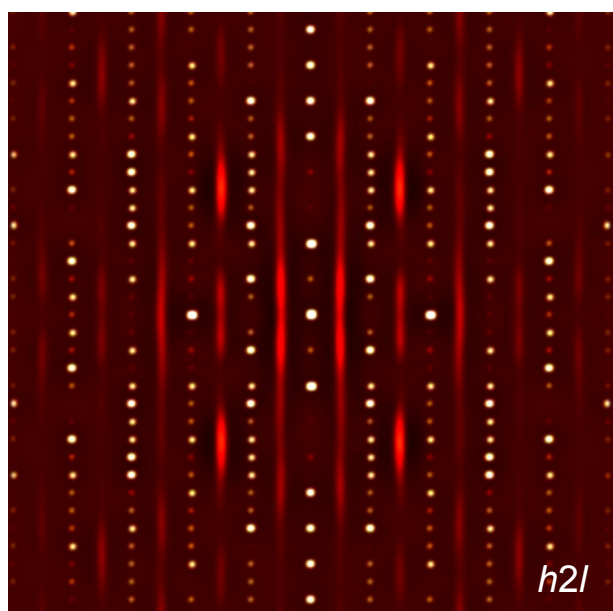
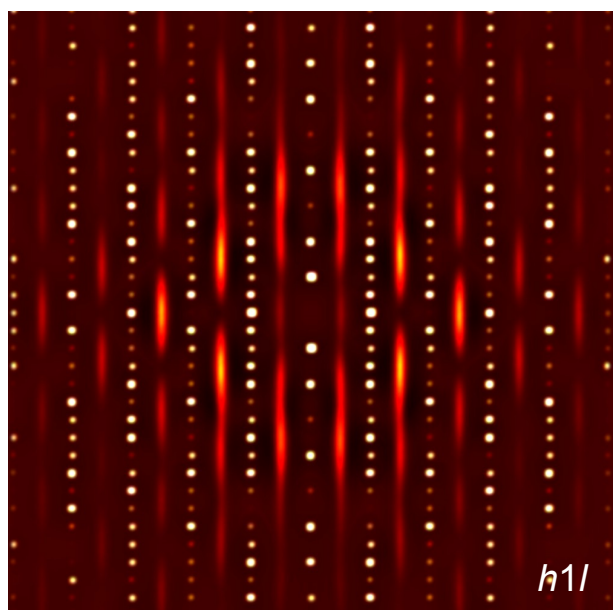


Figure 5. Calculated sections of reciprocal space for 2-D model with interaction parameters $J_I^a = 2$ and $J_I^c = 0$.

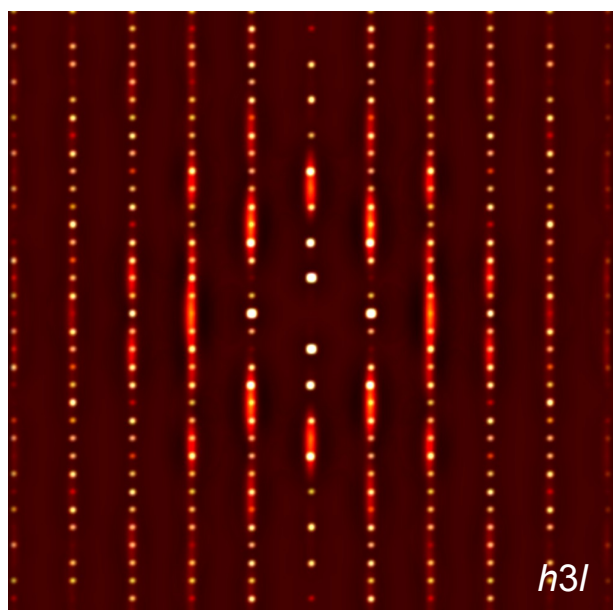
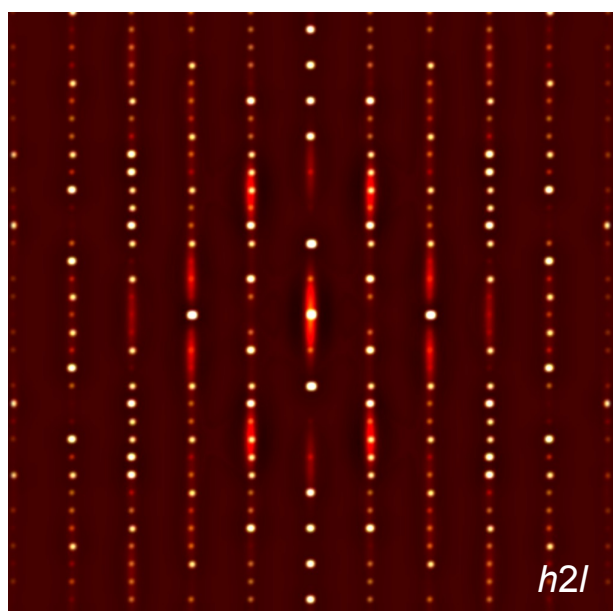
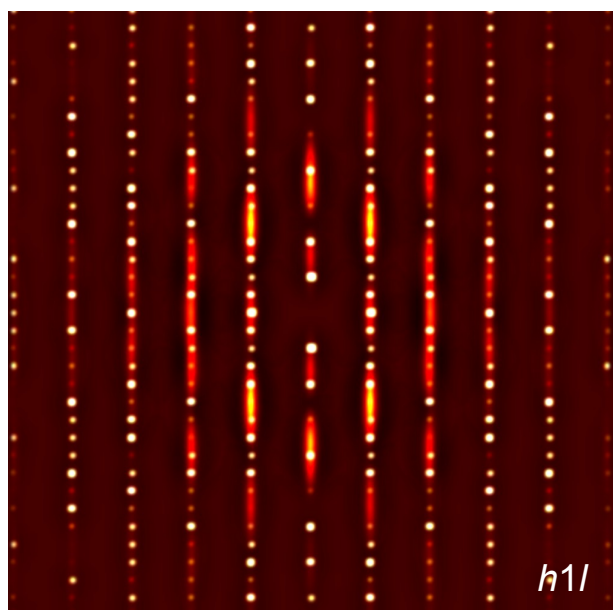


Figure 6. Calculated sections of reciprocal space for 2-D model with interaction parameters $J_I^a = -2$ and $J_I^c = 0$.

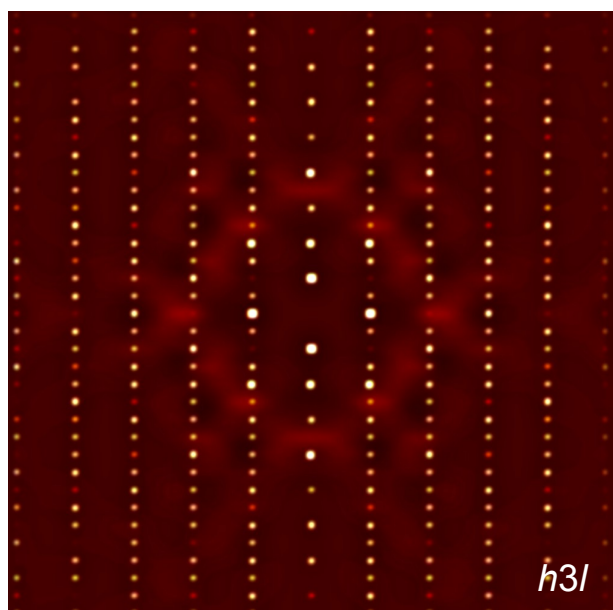
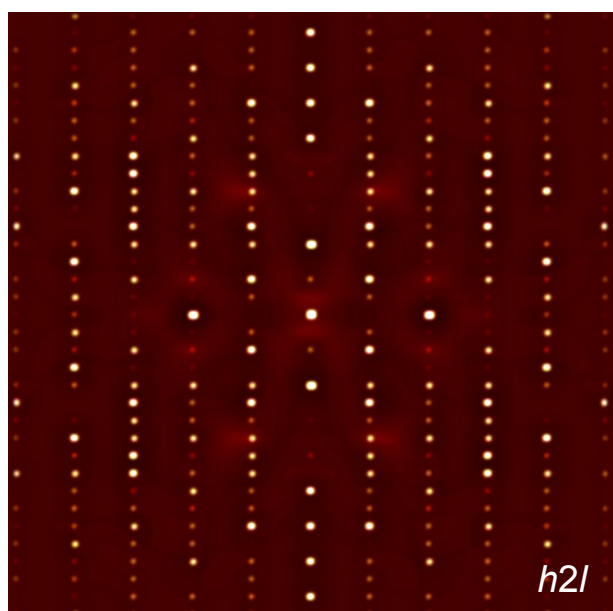
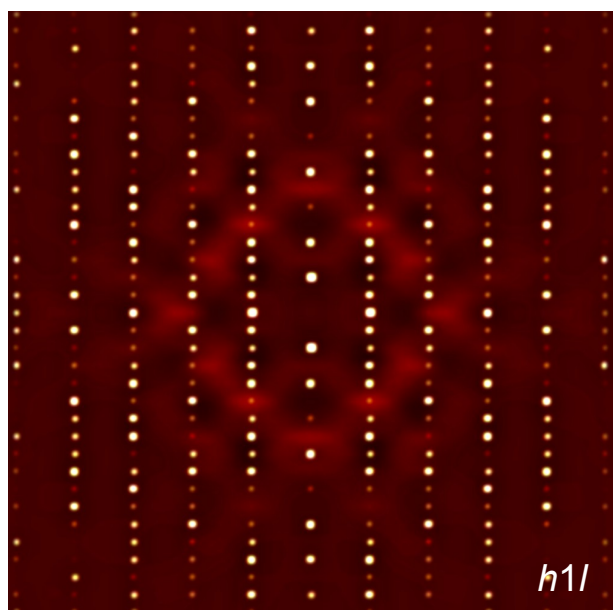


Figure 7. Calculated sections of reciprocal space for 2-D model with interaction parameters $J_I^a = 0$ and $J_I^c = -0.22$.

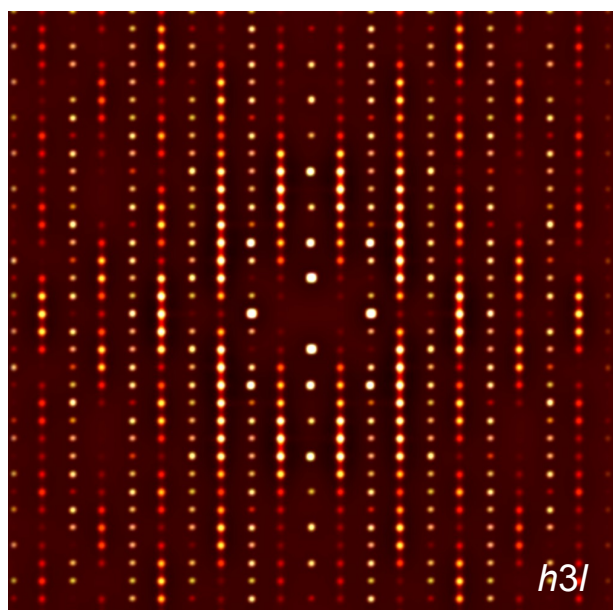
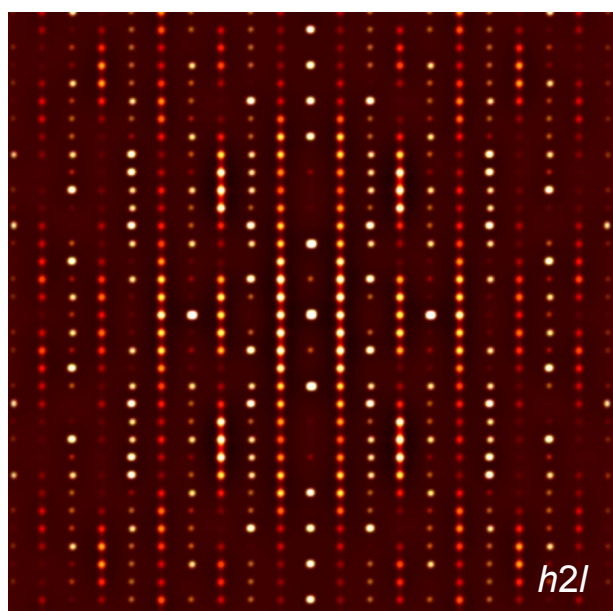
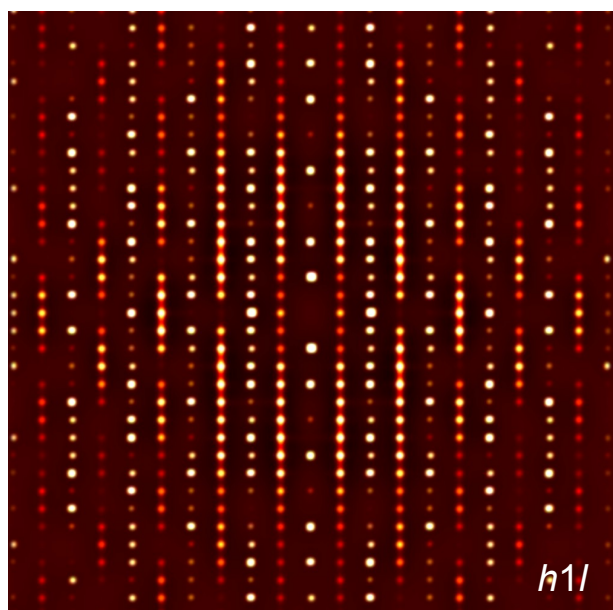


Figure 8. Calculated sections of reciprocal space for 2-D model with interaction parameters $J_I^a = 5$ and $J_I^c = -0.22$.