Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

The PBC network diagrams of important crystal faces of NTO were showed in Fig. 1.

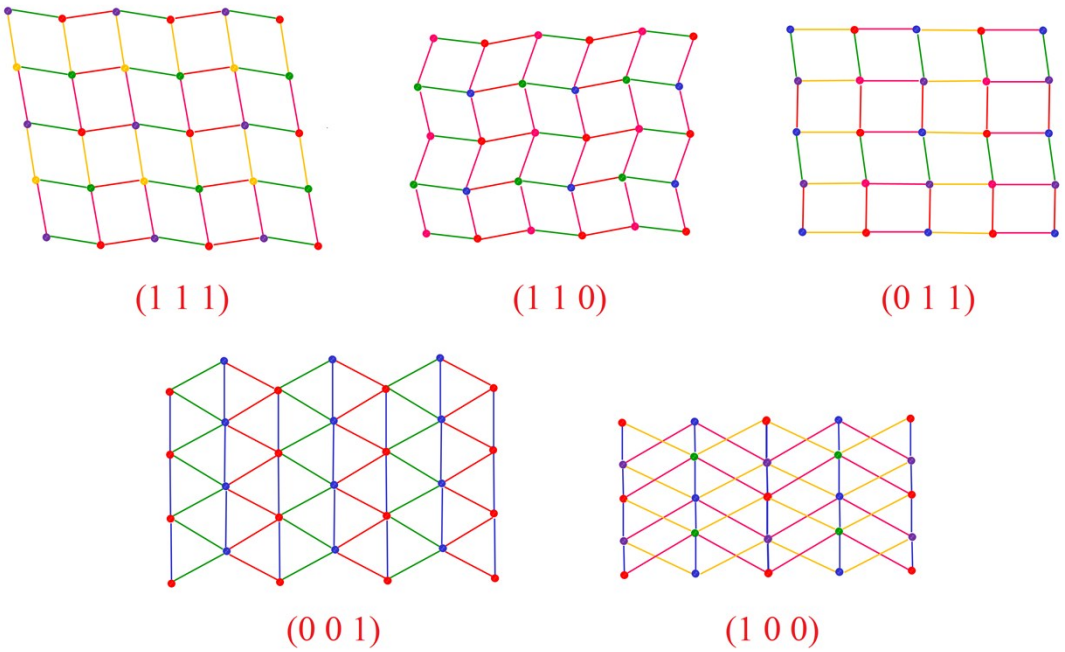

Fig. 1 The PBC network diagram was sliced in the direction of important crystal faces.

PBC diagrams are used to display the network of intermolecular interactions occurring for each molecule. The connected nets are shown in Fig. 1. Circles represent centers of mass colored by the growth units, and lines represent centers of mass colo1red by strength. Table 1 lists the bond length between each molecular center less than 7 Å. The crystal growth rate is proportional to *E*S att. The higher the *E*S att in the crystal face, the more easily the face is to grow, and its importance is poor in crystal morphology. The attachment energy is proportional to the number of strong bonds on the direction perpendicular to the face.

The simulation details of confirming the model size (d_c, d_s, d_v, U, V) are depicted in Fig. 2 to Fig. 6.

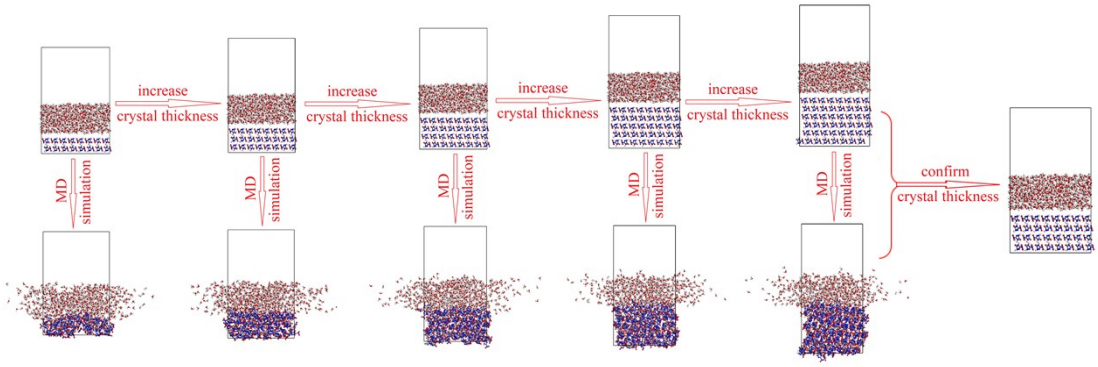

Fig. 2 Simulation details of confirming the crystal thickness.

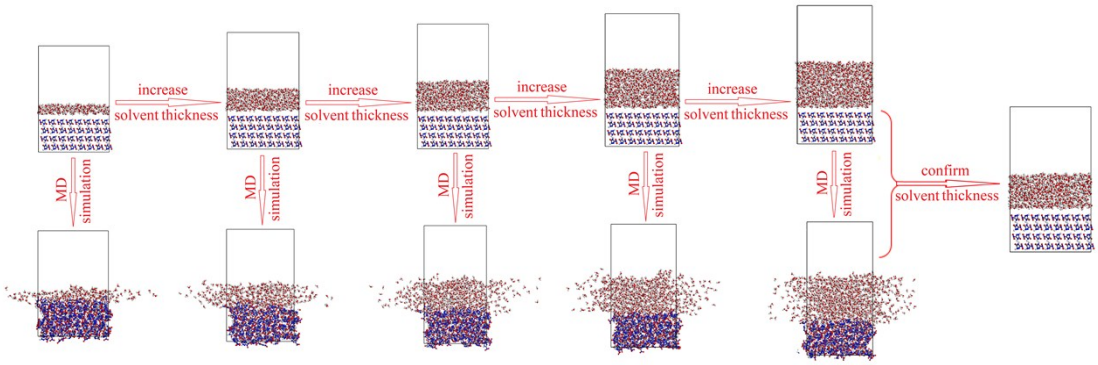

Fig. 3 Simulation details of confirming the solvent thickness.

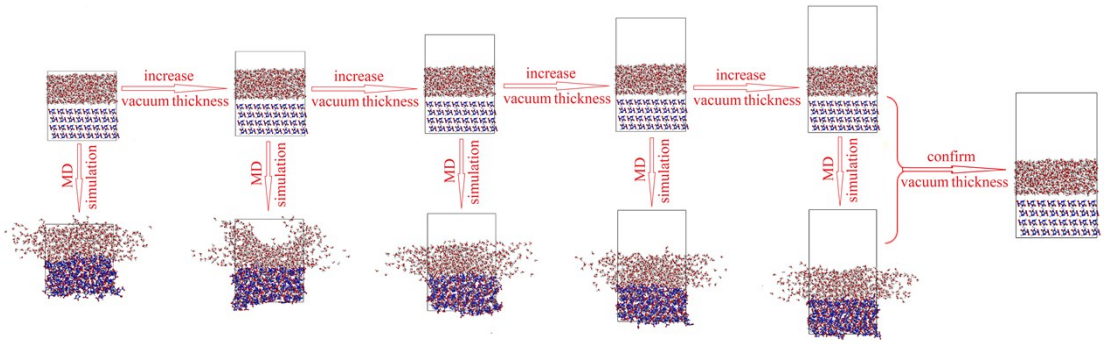

Fig. 4 Simulation details of confirming the vacuum thickness.

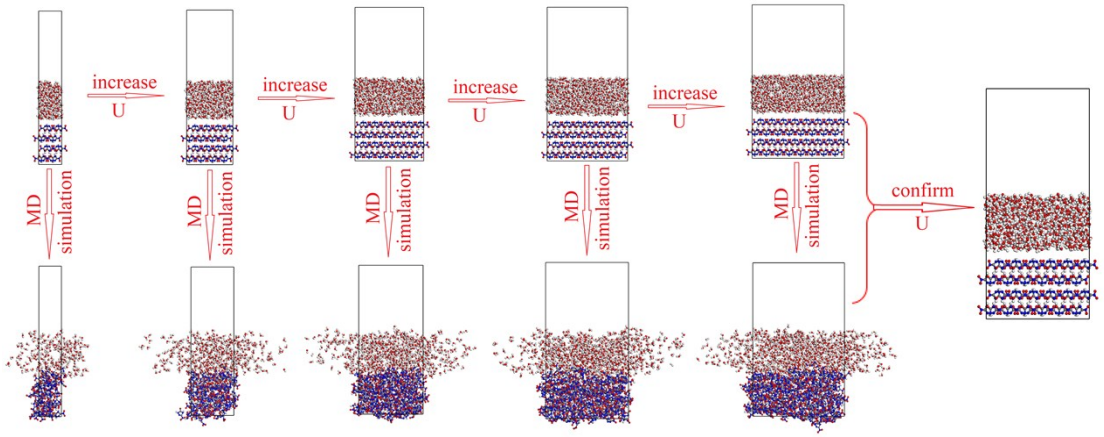

Fig. 5 Simulation details of confirming the U.

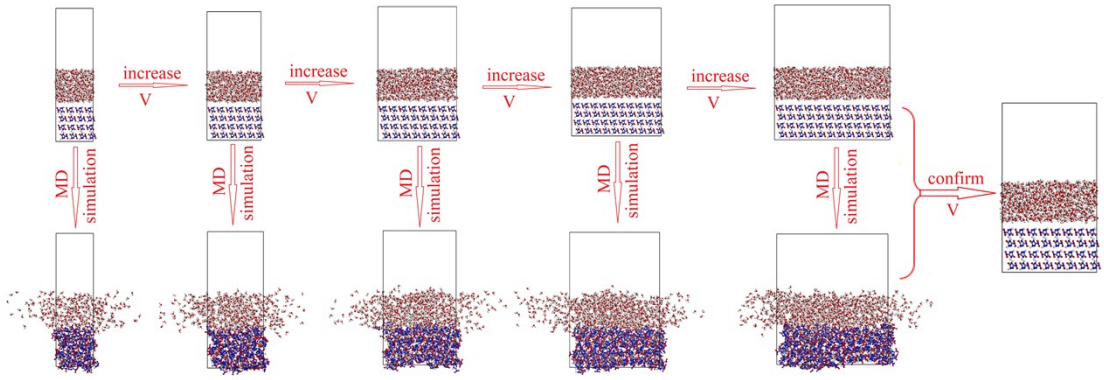

Fig. 6 Simulation details of confirming the V.