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# Solvent selection for explaining the morphology of nitroguanidine crystal by molecular dynamics simulation

Liang Song, Lizhen Chen,* Duanlin Cao, Jianlong Wang

School of Chemical Engineering and Environment, North University of China, Taiyuan 030051, *PR* China

Highlights

1. We predict NQ crystal morphology in different solvents using the MAE model.
2. The PBC and ESP on important morphological faces were analyzed.
3. We explain the mechanism of solvent effects on the crystal surface structure.
4. Interaction energy is used to explain the influence of the different solvents.

**ABSTRACT:** In this article, a method was performed to predict the morphology of needle-shaped crystals by analyzing the growth mechanisms for the various crystal faces. As an example, the crystal morphology of a nitroguanidine (NQ) was investigated via molecular dynamics simulations. The modified attachment energy (MEA) model was constructed by introducing surface chemistry terms and the relevant morphology of the habit crystal faces. The results indicate that the growth morphology of NQ in vacuum is dominated by {220}, {040}, {111}, {131} and {311} faces. The {220} and {040} faces are parallel to the elongation direction of the crystal, while the other faces are at the needle tips direction. The atoms or atomic groups exposed in crystal surface were used to analyze the relationship between structure and morphology. Compared to the surrounding faces, the needle tip faces have a large number of polar atoms or atomic groups. The needle tip faces have a high electronegativity on N, O atoms via molecular electrostatic potential (ESP) analysis. Furthermore, the protic solvent was used to reduce the attachment energy of the tip surfaces for achieving the purpose of inhibiting the growth of needle tips. Gamma-butyrolactone as the selected solvent inhibited effectively the growth of the needle tip faces. The predicted result is serviceable for the formation design.

* Corresponding author. Tel.: +86 13934510343. *E-mail address:* chen17555@163.com (Lizhen Chen)