几种极性有机晶体的生长习性与形成机理

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摘要 有机晶体特别是极性有机晶体,在不同的溶剂中具有明显不同的生长习性。本文通过对4-氨基-4'-硝基二苯硫醚(ANDS)等几种典型极性有机晶体在不同溶剂中的生长习性和结晶形貌的讨论,提出了偶极生长基元叠合模型,从两个方面探讨了这些习性的形成机理,即(1)有机晶体在不同的溶剂中具有不同结构和形式的生长基元(对于极性有机晶体而言,这些生长基元都具有偶极子特征),而不同的生长基元往晶体的各个面族上叠合的相对速率不同,从而导致了晶体习性的改变;(2)晶体生长界面的性质不同,特别是对于极性晶体,晶体界面的极性不同;不同的溶剂与生长晶体的界面相互作用不同,即使同种溶剂对晶体不同界面上的作用也不同,因而改变了生长界面的性质,影响了生长基元在晶体界面,特别是晶体正、负极面上的叠合速率,从而导致了晶体形貌的变化。由此比较合理地解释了晶体所呈现的不同的生长习性,特别是合理地解释了极性有机晶体所呈现的极性生长特征。

关键词 晶体生长 溶剂效应 硫醚 P 极性

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Growth habits and mechanism of several polar organic crystals in various solvents

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Abstract Growth habits of several polar organic crystals with a structure A-C6H4-D such as 4-amino-4'-nitrodiphenyl sulfide (ANDS), o-dicyanovinyl anisole (DIVA), N-4-nitrophenyl-(L)-prolinol (NPP) and 2-methyl-4-nitroaniline (MNA) depend strongly on the solvents from which they are grown. An incorporation model of polar growth units has been proposed to qualitatively explain the observed growth forms, which was based on: (1) the influence of the interaction between the solvent molecules and the growth units on the structural forms of the growth units; and (2) the interaction between the solvent molecules and the growth interfaces, particularly two polar faces for polar organic crystals. Since these interactions strongly affect the incorporation rates of the growth units on the positive and negative faces, a variety of the crystal habits such as polar growth, needle habits or platelet forms appear, and thus a good explanation for the observed habits in various solvents is expected to be obtained.

Key words CRYSTAL GROWTH SOLVENT EFFECT SULFUR ETHER P POLARITY

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