

研究论文

羧酸共聚物与方解石晶体相互作用的MD模拟

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收稿日期 2005-9-29 修回日期 2006-2-13 网络版发布日期 2006-9-8 接受日期 2006-5-8

**摘要** 用分子动力学方法, 模拟计算了丙烯酸-丙烯酸甲酯共聚物(AA-MAE)、丙烯酸-丙烯酸羟丙酯共聚物(AA-HPA)、丙烯酸-马来酸共聚物(AA-MA)及水解马来酸酐(HPMA)四种聚羧酸类阻垢剂与方解石晶体(110)晶面的相互作用. 结果表明, 聚羧酸与(110)晶面结合能的大小排序为AA-MA > HPMA > AA-HPA > AA-MAE; 对体系各种相互作用以及径向分布函数的分析表明, 结合能主要由库仑作用(包括离子键)提供, 并含少量氢键成分. 与方解石晶面结合的聚合物发生扭曲变形, 但形变能远小于相应的非键作用能. 聚合物中不同位置羧基的动力学行为差别很大, 链端羧基的运动翻转比链中部羧基剧烈得多, 故后者与晶面的结合比前者更牢固而具有更强的阻垢能力.

**关键词** [分子动力学](#) [羧酸共聚物](#) [方解石](#) [结合能](#) [形变能](#) [径向分布函数](#)

分类号

**Molecular Dynamics Simulation of Interaction between Carboxylate Copolymer and Calcite Crystal**

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**Abstract** This paper mainly simulates the interactions, in way of molecular dynamics, between four kinds of carboxylate copolymers, such as acrylic acid-methyl acrylate copolymer (AA-MAE), acrylic acid- 2-hydroxypropyl acrylate copolymer (AA-HPA), acrylic acid-maleic acid (AA-MA), hydrolysed polymaleic anhydride (HPMA) and (110) crystal surface of calcite crystal. The results show that the orders of binding energy of the four polymers with (110) crystal surface are as follows: AA-MA > HPMA > AA-HPA > AA-MAE, while the analysis of various interactions and radial distribution functions of all systems indicates that binding energies are mainly provided by coulomb interaction including electrovalent bond and a spot of hydrogen bond. Polymers were deformed during their combination with calcite crystal surfaces, with the deformation energies of polymers far less than respective nonbond energies. The dynamics behaviors of carboxyls at different positions of polymer chains are widely different. Carboxyls at the end of chains oscillate more rapidly than those in the middle, therefore the middle ones have more effective scale inhibitor ability than the end segments because they combine with calcite crystal more firmly.

**Key words** [molecular dynamics](#) [carboxylate copolymer](#) [calcite](#) [binding energy](#) [deformation energy](#) [radial distribution function](#)

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