Molecular dynamics simulation of dielectric polymers

2004 Fiscal Year Final Research Report Summary

Molecular dynamics simulation of dielectric polymers

Research Project

Project/Area Number

15607009

Research Category

Grant-in-Aid for Scientific Research (C)

Allocation Type

Single-year Grants

Section

一般

Research Field

計算科学

Research Institution

KANAZAWA UNIVERSITY

Principal Investigator

HIWATARI Yasuaki Kanazawa Univ., Natural Science & Technology, Professor, 自然科学研究科, 教授 (20019491)

Project Period (FY)

2003 – 2004

Keywords

molecular dynamics simulation / dielectric properties / polymers

Research Abstract

Application of molecular dynamics simulation to industry is another important role in addition to various basic researches in science and technology. Two examples have been studied here.
(1)A molecular dynamic study of a nanoparticle-composite polymer has been carried out to investigate key parameters which control fundamental properties of polymers such as glass transition temperature, thermal expansion coefficient, specific heat etc.
(2)The second study is one for the material design of dielectric polymers, such as a portable phone in near future which works in a much higher frequency domain than presently used one and consequently makes possible faster and more massive communication at once. For these purposes we study here complex dielectric properties of a polymer by molecular dynamics simulations. As far as the dielectric constant is concerned, the charge distribution of polymers is essential. However the introduction of charges into any molecular simulation systems must be a time ⋯▾ More