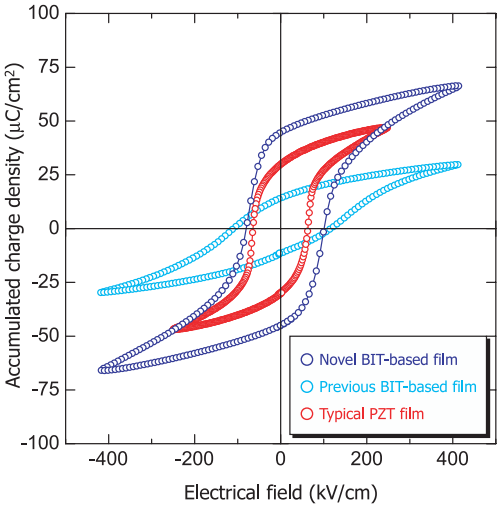
Development of Environment-Friendly Ferroelectric Films

- Toward top performance ferroelectric memory and piezoelectric microdevices -

Hirofumi MATSUDA
Smart Structure Research Center
e-mail: hiro-matsuda@aist.go.jp
AIST Today Vol. 3, No.12 (2003) 20

Novel synthesis technology for ferroelectric thin films on silicon has been developed. The film ensures both lead-free, environment-friendly composition and superior performance to lead-containing films that are strongly demanded for the replacement of lead-based materials. We have focused on the base material of $Bi_4Ti_3O_{12}$ (BIT) layer-structured crystal that has been attracting vast interest particularly in non-volatile ferroelectric memory field. To BIT, we have applied our novel design concept of film synthesis with optimization of atomic arrangement of underlying substrate beneath the film and modification of growth rate of atomic planes in BIT structure by Bi-site substitution and succeeded for the first time in revealing ideal ferroelectric property of perfect BIT single crystal.

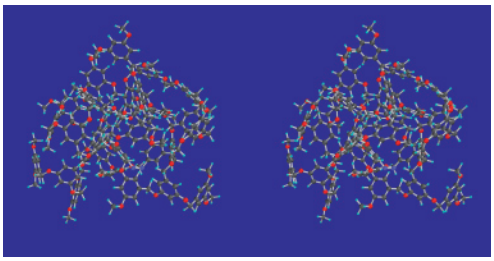


Superior ferroelectric property in novel BIT-based films

Development of ab initio Molecular Simulation System

Tsutomu IKEGAMI
Grid Technology Research Cetnter
e-mail: t-ikegami@aist.go.jp
AIST Today Vol. 3, No.12 (2003) 23

The ab initio molecular simulation system was developed, in which non-empirical methods such as the molecular orbital theory are used to evaluate a force field. Because no *a priori* informations are needed such as chemical bondings and/or atomic partial charges, it can cover most of the chemical systems. The simulation program is parallelized by using the grid technology, which enables us to run simulations using several remote computers in a unified manner.



Stereogram of aryl ether dendrimer obtained from the REXMC simulation