

Theory and Computer Experiments of the Slow Dynamics in Random Mediums

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1994 Fiscal Year Final Research Report Summary

Theory and Computer Experiments of the Slow Dynamics in Random Mediums

Research Project

Project/Area Number

05640439

Research Category

Grant-in-Aid for General Scientific Research (C)

Allocation Type

Single-year Grants

Research Field

物性一般(含基礎論)

Research Institution

Kanazawa University

Principal Investigator

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Co-Investigator(Kenkyū-buntansha)

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Project Period (FY)

1993 – 1994

Keywords

Supercooled Fluid / Glass Transition / alpha Relaxation / beta Relaxation / Non-Gaussian Transition / Anomalous Diffusion / Charged Polymer Chain

Research Abstract


Using 2-dimensional and 3-dimensional soft-sphere models, we have carried out molecular dynamics simulations for their supercooled fluid states. It has been shown that there are at least two different types of jumping motions of atoms in highly supercooled states and possibly glassy states, one of which, corresponding to the smaller averaged jump rate, can be specified by a distribution of the jump rates rather than a constant jump rate.


These two jump motions are responsible to the alpha and beta slow dynamics in supercooled fluid states. Taking into consideration these two coarse-grained motions of atoms and trapping diffusion-type of equation (master equation) , we have found the following main results :
 (1) Quasi anomalous diffusion takes place in highly supercooled fluid states, leading to the anomalous dynamics in intermediate time scales known as alpha and beta relaxation of the density autocorrelation function. (2) Below the glass transition temperature anomalous diffusion takes place, namely the diffusion constant becomes zero. This indicates that the anomalous dynamics occurs in infinitely long time limit. The liquid-glass transition is specified in this theory by the Gaussian-to-non-Gaussian transition. (3) The above results are consistent with the behavior of the generalized susceptibility obtained by the molecular dynamics simulation, and with recent experiments.
 In addition, as a related problem, we have also studied a system of charged polymer melts (plus counter ions) using molecular-dynamics simulation.


Research Products (46 results)


		All	Other
		All	Publications (46 results)
[Publications]	J.Habasaki: "Glass Transition Temperatures Studied by MD Simulation of Some Alkali Metasilicates" Mol.Sim.10. 19-26 (1993)		▼
[Publications]	M.Takasu: "Numerical Studies of Electron Transfer" Proc.CAMSE'92. 375-378 (1993)		▼
[Publications]	J.Habasaki: "A Molecular-Dynamics Study on the Liquid-Glass Transition in Alkali Metasilicates" Proc.CAMSE'92. 251-254 (1993)		▼
[Publications]	Y.Hiwatari: "Study on Slow Dynamics of Highly Supercooled Liquids and the Liquid-Glass Transition via Molecular Dynamics Simulation" Proc.CAMSE'92. 241-246 (1993)		▼
[Publications]	M.Takasu: "Relaxation of Quantum Systems in a Fluctuating Medium" Quantum Monte Carlo Methods in Condensed Matter Physics,ed.M.Suzuki(World Scientific,Singapore). 355-368 (1993)		▼
[Publications]	S.Itoh: "Dynamical Singularity of the Glass Transition in Molten Lithium Iodide" Non-Cryst.Solids. 156-158. 559-563 (1993)		▼
[Publications]	J.Matsui: "Calculation of the Generalized Susceptibility for a Highly Supercooled Fluid through Molecular-Dynamics Simulation" Mol.Sim. 12. 305-316 (1993)		▼
[Publications]	Y.Hiwatari: "Study of the α and β relaxations in a Supercooled Fluid via Molecular-Dynamics Simulation" Physica A. 204. 306-327 (1994)		▼
[Publications]	K.Uehara: "Molecular-Dynamics Simulations for the Density Autocorrelation Function in a Supercooled Fluid Phase" Mol.Sim.12. 253-270 (1994)		▼
[Publications]	T.Odagaki: "Trapping Diffusion Model for Glass Transition and Slow Dynamics in Supercooled Liquids" Physica A. 204. 464-481 (1994)		▼
[Publications]	T.Odagaki: "The Role of Molecular Dynamics Simulations for the Study of Slow Dynamics" Mol.Sim. 12. 299-304 (1994)		▼
[Publications]	S.Kambayashi: "Molecular-Dynamics Study of Dynamical Properties of Dense Soft-Sphere Fluids:" Phys.Rev.E. 49. 1251-1259 (1994)		▼
[Publications]	T.Hasegawa: "Dynamical Properties of Condensed Charged Polymer Melts" Mol.Sim.12. 356-381 (1994)		▼
[Publications]	T.Muranaka: "Molecular-Dynamics Study of the Diffusion of Hydrogen in Solid Palladium" Mol.Sim.12. 329-341 (1994)		▼
[Publications]	J.Matsui: "Study of the Slow Dynamics in a Highly Supercooled Fluid:Super-Long-Time Molecular Dynamics Calculation of the Generalized Susceptibility" Phys.Rev.Letters. 73. 2452-2455 (1994)		▼
[Publications]	T.Odagaki: "Slow Dynamics in Supercooled Liquids" Phys.Rev.E. 49. 3150-3158 (1994)		▼
[Publications]	T.Muranaka: "A Study of the β Relaxation in a Highly Supercooled State via Molecular-Dynamics Simulation" Phys.Rev.E. (印刷中).		▼


[Publications] S.Itoh: "Dynamical Singularity of the Glass Transition on Molten Lithium Iodide" Proc.LAM8. (印刷中).	▼
[Publications] 樋渡保秋: "ガラス転移研究の最近の発展" 計算物理学ニュースレター. 7. 18-29 (1994)	▼
[Publications] 樋渡保秋: "分子動力学法を用いた複雑系の研究" 第15回日本熱物性シンポジウム. 385-388 (1994)	▼
[Publications] S.Kambayashi: "Numerical Calculation of the Bridge Function for Soft-Sphere Supercooled Fluids via Molecular Dynamics Simulations" Mol.Sim.12. 421-430 (1994)	▼
[Publications] T.Odagaki: "Glass Transition Singularities and Slow Dynamics" Proc.MRS meetings. (印刷中).	▼
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[Publications] Y.Hiwatari: "Molecular-Dynamics Study of Supercooled Liquids and the Theory of the Glass Transition" J.Phys.Soc.Jpn.Supplement. (印刷中).	▼
[Publications] J.Habasaki et.al.: "Glass Transition Temperatures Studied by MD Simulation of Some Alkali Metasilicates" Mol.Sim.10. 19-26 (1993)	▼
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[Publications] S.Kambayashi et.al.: "Molecular-Dynamics Study of Dynamical Properties of Dense Soft-Sphere Fluids : The Role of Short-Range Repulsion of the Intermolecular Potential" Phys.Rev.E49. 1251-1259 (1994)	▼
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[Publications] T.Muranaka et.al.: "A Study of the beta Relaxation in a Highly Supercooled State via Molecular-Dynamics Simulation" Phys.Rev.E. (in press).	▼
[Publications] S.Itoh et.al.: "Dynamical Singularity of the Glass Transition on Molten Lithium Iodide" Proc.LAM8. (in press).	▼

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[Publications] Y.Hiwatari et.al.: "Slow Dynamics in Supercooled Flu" J.Mol.Liquids. (in press). 

[Publications] Y.Hiwatari et.al.: "Molecular-Dynamics Study of Supercooled Liquids and the Theory of the Glass Transition" J.Phys.Soc.Jpn.Supplement. (in press). 

[Publications] M.Takasu: "Relaxation of Quantum Systems in a Fluctuating Medium" , in Quantum Monte Carlo Methods in Condensed Matter Physics, ed.M.Suzuki. World Scientific, Singapole, 355-368 (1993) 

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