

# Structures and Dynamics of Amorphous Alloys

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# 1991 Fiscal Year Final Research Report Summary

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## Structures and Dynamics of Amorphous Alloys

Research Project

### Project/Area Number

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01540294

### Research Category

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

### Allocation Type

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Single-year Grants

### Research Field

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物性一般（含極低温・固体物性に対する理論）

### Research Institution

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Kanazawa University

### Principal Investigator

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### Project Period (FY)

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1989 – 1991

### Keywords

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Dynamics near Liquid-Glass Transition / Dynamics of binary Supercooled Liquids / Density Fluctuations in Supercooled Liquids / Anomalous Non-Gaussian Behavior / Jump Diffusion / Trapping Diffusion Model / Theory of Pair Distribution Function in Liquids / Short Range Interaction and Phase Separation

### Research Abstract

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1. Anomalous Dynamics near Liquid-Glass Transition : On approaching a liquid-glass transition, the relaxation time of density fluctuations in a supercooled liquid becomes extremely long. With this dynamical slowing down, various anomalous properties are observed in highly supercooled liquids. Then, we have studied atomic-level mechanisms as well as dynamical structures of highly supercooled liquids, using a simple binary alloy model, for which molecular dynamics(MD)simulations have been carried out. Main results obtained are (1)the density autocorrelation functions in highly supercooled liquids are well fitted by a stretched exponential function, (2)the atomic diffusion takes place mainly through jump motions correlated with several nearby atoms, (3)non-Gaussian parameter(NGP)becomes unusually large compared with that of normal liquid states, (4)the maximum of the NGP times the corresponding time makes it possible to estimate the liquid-glass transition ; one of the most advantage of this method is that the glass transition can be determined by an intermediate time behavior rather than long time behavior like self-diffusion, and (5)the

exponent of the stretched exponential function stated in(1)depends on the temperature(density), so that this result disagrees with that of the simplest version of mode coupling models.

2. Theory of Slow Dynamics near the Glass Transition : With a trapping diffusion model, we have studied dynamical properties of supercooled liquids, which turns out to be consistent with the present MD results.

3. Theory of Pair Distribution Functions for Supercooled Liquids : With an improved integral equation(MHNCS), we have obtained an interesting result on the effect of a short range repulsive interaction on the phase separation of binary mixtures.

# Research Products (26 results)

		All	Other
		All	Publications (26 results)
[Publications]	T.Odagaki and Y.Hiwatari: ""Gaussian-to-non-Gaussian Transition in Supercooled Fluids"" Phys.Rev. A43. 1103-1106 (1991)		▼
[Publications]	Y.Hiyatari,H.Miyagawa and T.Odagaki: ""Dynamical Singularities near the Liquid-Glass Transition:Theory and Molecular Dynamics Study"" Solid State Ionics. 47. 179-222 (1991)		▼
[Publications]	樋渡 保秋,宮川 博夫,小田 垣孝: ""ガラス転移の疑似動的臨界現象"" 日本物理学会誌. 46. 90-97 (1991)		▼
[Publications]	J.Takashima,M.Takasu and Y.Hiwatari: ""Equilibrium Properties of a Charged Polymer Chain with Short Range Interactions:Two-Dimensional Monte Carlo Studies"" Mol.Simulation. 6. 199-220 (1991)		▼
[Publications]	M.Takasu,K.Uehara,T.Muranaka and Y.Hiwatari: ""Molecular Dynamics Study of PdH_X System"" Proc.Int.Workshop on Computational Materials Science,NRIM,Tsukuba,Aug.23-24. 203-206 (1990)		▼
[Publications]	T.Odagaki and Y.Hiwatari: ""Residence Time Distribution of a Tracer Atom in Supercooled Fluids"" J.Phys.:Condens.Matter. 3. 5191-5194 (1991)		▼
[Publications]	H.Miyagawa,Y.Hiwatari and S.Itoh: ""Molecular-Dynamics Study for the Glass Transition in LiI"" Prog.Theor.Phys.,Supplement. 103. 47-60 (1991)		▼
[Publications]	Y.Hiwatari,H.Miyagawa,T.Muranaka and K.Uehara: ""Molecular-Dynamics Study of Highly Supercoole*d Liquids:Dynamical Singularities near the Liquid-Glass Transition"" Proc.Tohwa University International Symposium on Slow Dynamics in Condensed Matter,edited by M.Tokuyama (AIP,New York). (1992)		▼
[Publications]	T.Odagaki and Y.Hiwatari: ""Stochastic Dynamics in a supercooled Fluid"" Proc.Tohwa University International Symposium on Slow Dynamics in Condensed Matter,edited by M.Tokuyama (AIP,New York). (1992)		▼
[Publications]	S.Kambayashi and Y.Hiwatari: ""Instability and Phase Separation of a Binary Mixture:The role of Short-Range Repulsion and Core-Size Ratio"" Phys.Rev.A. (1992)		▼
[Publications]	J.Habasaki,I.Okada and Y.Hiwatari: "A Molecular Dynamics Study for Lithium Metasilicate:Liquid and Quenched Supercooled States"" Mol.Simulation. (1992)		▼
[Publications]	H.Miyagawa and Y.Hiwatari: ""Molecular-Dynamics Study of the Glass Transition in a Binary Soft-sphere Model"" Phys.Rev. A44. 8278-8288 (1991)		▼
[Publications]	T.Odagaki and Y.Hiwatari: ""Apparent Subdiffusive Properties of a Supercooled Fluid"" Phys.Rev.A. (1992)		▼
[Publications]	T. Odagaki and Y. Hiwatari: ""Gaussian-to-non-Gaussian Transition in Supercooled Fluids"" Phys. Rev.A43. 1103-1106 (1991)		▼
[Publications]	Y. Hiwatari, H. Miyagawa and T. Odagaki: ""Dynamical Singularities near the Liquid -Glass Transition : Theory and Molecular Dynamics Study"" Solid State Ionics. 47. 179-222 (1991)		▼
[Publications]	Y. Hiwatari, H. Miyagawa and T. Odagaki: ""Quasi Critical Dynamics Phenomena near Liquid-Glass Transition (in Japanese)"" J. Jpn. Phys. Soc.46. 90-97 (1991)		▼

- [Publications] J. Takashima, M. Takasu and Y. Hiwatari: ""Equilibrium Properties of a Charged Polymer Chain with Short Range Interactions : Two-Dimensional Monte Carlo Studies"" Mol. Simulation. 6. 199-220 (1991) ▼
- [Publications] M. Takasu, K. Uehara, T. Muranaka and Y. Hiwatari: ""Molecular Dynamics Study of PdHchi System"" Proc. Int. Workshop on Computational Materials Science, NRIM. 203-206. (1991) ▼
- [Publications] T. Odagaki and Y. Hiwatari: ""Residence Time Distribution of a Tracer Atom in Supercooled Fluids"" J. Phys. : Condens. Matter. 3. 5191-5194 (1991) ▼
- [Publications] H. Miyagawa, Y. Hiwatari and S. Itoh: ""Molecular-Dynamics Study for the Glass Transition in LiI"" Prog. Theor. Phys., Supplement. 103. 47-60 (1991) ▼
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- [Publications] S. Kambayashi and Y. Hiwatari: ""Instability and Phase Separation of a Binary Mixture : The role of Short-Range Repulsion and Core-Size Ratio"" Phys. Rev. A. ▼
- [Publications] J. Habasaki, I. Okada and Y. Hiwatari: ""A Molecular Dynamics Study for Lithium Metasilicate : Liquid and Quenched Supercooled States"" Mol. Simulation. ▼
- [Publications] H. Miyagawa and Y. Hiwatari: ""Molecular-Dynamics Study of the Glass Transition in a Binary Soft-Sphere Model"" Phys. Pev.A44. 8278-8288 (1991) ▼
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