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6. AUTHOR(S) S. J. Poon and G. J. Shiflet	DTIC SELECTE S G D
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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) University of Virginia Department of Physics McCormick Road Charlottesville, VA 22901	8. PERFORMING ORGANIZATION REPORT NUMBER 9 1991
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13. ABSTRACT (Maximum 200 words)  
We have synthesized a new class of metallic glasses based on aluminum. The unusual structural and formality of these glasses have been investigated by x-ray and neutron diffraction, and by high-resolution electron lattice imaging experiments. The glassy nature is confirmed and a dense-random-packing of rare-earth atoms is observed. This new class of aluminum-based metallic glasses has low density, high tensile strength, and good corrosion-resistant properties which are important for technological applications. We have also performed extensive structural studies of icosahedral and decagonal crystals. Diffraction measurements have been compared with atomic models proposed for quasicrystals. It is found that the decoration of Penrose tiling provides an adequate description of experimental findings in icosahedral crystals. In the case of decagonal crystals, there is strong evidence for an entropy stabilization mechanism. Structural defects in complex crystals closely related to icosahedral crystals have been studied. The defects have been found to be of the planar type and their structure forms the basis of icosahedral phase formation.

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UNCLASSIFIED

## Rapidly Solidified Metallic Alloys with Unusual Symmetry Properties

### Statement of the problem studied:

The objectives of our program are to synthesize new metastable alloys by rapid solidification, to study their thermal stability and unusual symmetry properties, and to relate findings to their structural counterparts. Structures of new materials are investigated by neutron, x-ray and electron diffraction, including that of high-resolution diffraction. Alloy systems having relevance to magnetic and mechanical applications are chosen for study.

### Summary of the most important results:

(1) Discovery of glassy aluminum alloys containing up to 90 at.% aluminum -

While searching for very aluminum-rich quasicrystals in the  $Al_{20}Fe_2Ce$  system, a single-phase metallic glass was discovered. In the field of metallic glasses, the difficulty in making amorphous aluminum-based alloys has been known for almost twenty years. Even more unexpected is the formation of glassy aluminum containing up to 90 at.% aluminum in systems where an eutectic region does not even exist. For glass forming systems known to date, metallic glasses containing as much as 90 at.% of one of the components are rarities; and the glassy phases can only be formed near the eutectic regions. The unusually high strengths of aluminum glasses can be of significant importance in obtaining high strength low density materials.

(2) Atomic scale structure of aluminum glasses -

We have studied the structural properties of aluminum-based metallic glasses by means of diffraction and thermal measurements. These studies have helped to resolve the longstanding controversies between the amorphous and microcrystalline models in metallic glasses. High resolution electron microscopy (HREM) experiments indicate amorphousness on the subnanometer scale. Calorimetric measurements indicate a nucleation and growth process during crystallization.

In collaboration with Professor T. Egami's group at U. Penn, the atomic structure of Al-Fe-Ce containing 90 at.% Al has been studied by x-ray and neutron scattering measurements. From radial

distribution analysis, it can be concluded that a significant portion of Al-Fe distances are shorter than the sum of Al + Fe radii, indicating a strong degree of s-d hybridization. On the other hand, some part of Al-Al distances are anonymously long. The analysis also shows that Ce atoms form a dense-random-packing glassy network. There is also a strong chemical and geometrical order around Fe. The configurational relationship of Ce with the "Al-Fe clusters" will be investigated further.

(3) Electrochemical properties of aluminum glasses -

Professor G. Stoner's group (Mat. Sci., UVA) has investigated the electrochemical properties of several of the Al-glasses. It is found that these glasses have exceptional corrosion-resistant properties at high pH (>9) values.

(4) Atomic scale structure of icosahedral crystals -

We have performed pulsed neutron scattering from single-phase  $\text{Al}_{55}\text{Cu}_{10}\text{Li}_{35}$ ,  $\text{Al}_{55}\text{Cu}_{10}\text{Li}_{30}\text{Mg}_5$ ,  $\text{Al}_{51}\text{Cu}_{12.5}\text{Li}_{23.5}\text{Mg}_{13}$  and  $\text{Al}_{51}\text{Cu}_{12.5}\text{Mg}_{36.5}$  alloys. Structure factors and pair distribution functions of these alloys are determined and from these the differential distribution functions of Mg and Li were derived. Al-Cu-Li and Al-Cu-Mg icosahedral phases are isostructural, except that small portion of Al(Cu) sites in Al-Cu-Li icosahedral phase are taken by Mg in Al-Cu-Mg icosahedral phase. Stable Al-Cu-Li i-phase has a better medium and long range order than the less stable Al-Cu-Mg i-phase. Our structure studies support the Henley-Elser structure model of  $(\text{Al,Zn})_{49}\text{Mg}_{32}$  type icosahedral phase. Successful structural models of icosahedral crystals should explain quantitatively the pair and differential distribution functions derived from our experiments. We are currently working on this.

Work in the Al-Cu-X systems include x-ray diffraction studies of the structure of the icosahedral and Frank-Kasper phases of  $\text{Al}_{5.5}\text{Li}_{3.3}\text{Cu}$ . It is shown that the two phases have very similar local structure up to about 20Å, while the long-range structure is quite distinct. A detailed analysis of the Frank-Kasper phase suggests that the reported atomic positions and site occupations of this compound are not accurate, and the local structure of this compound is actually closer to that of the quasicrystalline unit cells proposed for the icosahedral phase. The results are consistent with

the decorated quasicrystalline lattice model.

(5) Atomic scale structure of decagonal quasicrystals -

We have carried out high resolution electron-microscopy (HREM) studies and structure modeling of the stable decagonal phases of Al-Cu-Co. The images obtained by our group can be described by the tiling models; and they are similar to those observed by use of scanning tunneling microscopy (STM) at AT & T Bell Laboratories. These results are different from those of other decagonal phases such as Al-Fe and Al-Mn studied earlier. The latter systems show a very high degree of disorder in their lattice images. We have also carried out structural analysis by use of the "cut-and-projection" technique, that is, the lattice points in the two-dimensional quasicrystal are obtained by projecting points from the five-dimensional hypercubic space. It is found that there is strong evidence for an entropy stabilization mechanism in the Al-Cu-Co decagonal quasicrystal.

(6) Defect structures in the crystal-analog of quasicrystals -

Planar defects were found in the Frank-Kasper phase and imaged with atomic resolution electron microscopy. After computer analysis of the images the defects were found to be of {110} and {100} type planes. The faults are very narrow, in some cases only one lattice plane thick. To date no one has analyzed the defects in complex structures like the  $Al_5CuLi_3$ . We initiated this investigation because the defects in this structure may have some relationship to the  $Al_6CuLi_3$  icosahedral quasicrystal structure. It is observed that a feature common to many crystalline phases which are related to quasicrystals is this high density of planar defects. Because of the complex nature to their crystal structure, not much is known about the defects in these crystalline phases. A better understanding of the defects will provide information on the transformation from quasicrystalline to crystalline state, and therefore might help in understanding the formation of the quasicrystals.

**Publications Resulting From ARO Contract No. DAAL03-87K-0057**

**(only list refereed articles)**

1. W. Dmowski, T. Egami, Y. Shen, S. J. Poon, G. J. Shiflet, "Structural Relationship Between Icosahedral and Frank-Kasper Phases of Al-Li-Cu," *Phil. Mag. Lett.* 56, 63 (1987).
2. S. J. Poon, W. Dmowski, T. Egami, Y. Shen, and G. J. Shiflet, "Comparison of Quasicrystalline and Crystalline Structures in the Al-Cu-Li Using High-Resolution X-Ray Diffraction," *Phil. Mag. Lett.* 56, 259 (1987).
3. Y. Shen, W. Dmowski, T. Egami, S. J. Poon, and G. J. Shiflet, "Structure of Al-(Li, Mg)-Cu Icosahedral Alloys Studied by Pulsed Neutron Scattering," *Phys. Rev. B* 37, 1146 (1988).
4. Y. Shen, G. J. Shiflet, and S. J. Poon, "Stability and Formation of Al-Cu-(Li, Mg) Icosahedral Phases," *Phys. Rev. B* 38, 5332 (1988).
5. Y. He, S. J. Poon, and G. J. Shiflet, "Synthesis and Properties of Metallic Glasses That Contain Aluminum," *Science* 241, 1640 (1988).
6. G. Shiflet, Y. He, and S. J. Poon, "Mechanical Properties of Al-Fe-Gd Glasses," *Script. Met.* 22, 1661 (1988).
7. G. J. Shiflet, Y. He, and S. J. Poon, "Mechanical Properties of a New Class of Metallic Glasses Based on Aluminum," *J. Appl. Phys.* 64, 6843 (1988).
8. Y. He, S. J. Poon, and G. J. Shiflet, "Formation and Stability of Aluminum-Based Metallic Glasses in Al-Fe-Gd Alloys," *Script. Met.* 22, 1813 (1988).
9. Q. B. Yang, G. J. Shiflet, and S. J. Poon, "Shear Planes and Translation Domains in the  $Al_5CuLi_3$  Frank-Kasper Phase," *Phil. Mag. Lett.*, to be published (1991).
10. Y. He, H. Chen, G. J. Shiflet, and S. J. Poon, "On the Structural Nature of Aluminum-Based Metallic Glasses," *Phil. Mag. Lett.* 61, 297 (1990).
11. B. H. Toby, Y. He, J. D. Jorgensen, K. Volin, W. Dmowski, T. Egami, S. J. Poon, and G. J. Shiflet, "Atomic Structure of Amorphous Al-Fe-Ce Determined by Pulsed Neutron Scattering," published in *J. Mat. Res.*, Dec. (1990).

**Participating Scientific Personnel**

S. Joseph Poon - Principal Investigator

Gary J. Shiflet- Principal Investigator

K. R. Lawless - Principal Investigator

Y. Shen - Ph.D. awarded, August 1988

P. Diehl - M.S. awarded, May 1989

Y. He - Graduate Student (Ph.D)

H. Chen - Graduate Student (Ph.D)

**List of inventions:**

United States Patent (number 4, 964, 927) awarded on Oct. 23, 1990.

Title: Aluminum-Based Metallic Glass Alloys.



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1. NAME AND ADDRESS OF CONTRACTOR (Include Zip Code)  
Rector and Visitors, University of Virginia  
P.O. Box 9003  
Charlottesville, VA 22906

2. CONTRACT NUMBER  
DAAL03-87-K-0057

3. TYPE OF REPORT (Check One)

a. INTERIM  b. FINAL

4. INVENTION DATA (Listed below are all inventions required to be reported) (If "None," so state) **NONE**

(i) NAME OF INVENTOR(S)	(ii) TITLE OF INVENTION	(iii) CONTRACTOR DISCLOSURE IDENTIFICATION NUMBER OR PATENT APPLICATION SERIAL NUMBER	(iv) CONTRACTOR ELECTS TO FILE U. S. PATENT APPLICATION		(v) CONFIRMATORY LICENSE OR ASSIGNMENT FORWARDED TO CONTRACTING OFFICER	
			YES	NO	YES	NO
Gary J. Shiflet S. Joseph Poon Yi He	"Aluminum-Based Metallic Glasses"	4,964,927		✓		

5. SUBCONTRACT DATA (Listed is information required but not previously reported for Subcontracts) (If "None," so state) **NONE**

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**SECTION III - CERTIFICATION**

CONTRACTOR CERTIFIES THAT PROMPT IDENTIFICATION AND TIMELY DISCLOSURE OF SUBJECT INVENTIONS PROCEDURES HAVE BEEN FOLLOWED

NAME AND TITLE OF AUTHORIZED OFFICIAL (Print or Type)

D. Wayne Jennings, Director  
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