Project title: Nanostructure Determination by Co-Refining Models to Multiple Datasets

Principal investigator: Simon J. L. Billinge

Period the report covers: Sept. 1, 1997 – May 31, 2011

Name and address of recipient organization: Michigan State University, East Lansing, MI 48824

DOE award number: DE-FG02-97ER45651

Amount of unexpended funds: $0

Aims of the project: The aims of the project have not changed from the original application

Results of work to date:

The results of the work are contained in the publications resulting from the grant (which are listed below). Here I summarize the main findings from the last period of the award, 2006-2007:

- Published a paper in Science with Igor Levin outlining the "Nanostructure Problem", our inability to solve structure at the nanoscale.
- Published a paper in Nature demonstrating the first ever ab-initio structure determination of a nanoparticle from atomic pair distribution function (PDF) data.
- Published one book and 3 overview articles on PDF methods and the nanostructure problem.
- Completed a project that sought to find a structural response to the presence of the so-called "intermediate phase" in network glasses which appears close to the rigidity percolation threshold in these systems. The main result was that we did not see convincing evidence for this, which drew into doubt the idea that Ge_xSe_{1-x} glasses were a model system exhibiting rigidity percolation.

In addition to the published products listed below, Billinge gave 21 invited talks on this research during 2006-2007 (not listed explicitly). Two students supported by the grant also graduated with Ph.D's in this period, Ahmad Masadeh and Moneeb Shatnawi.

1. S. J. L. Billinge, **Local structure from total scattering and atomic pair distribution function (PDF) analysis**, In **Powder diffraction: theory and practice**, (Royal Society of Chemistry, London England, 2008), Robert E. Dinnebier and Simon J. L. Billinge, Eds., pp. 464 - 493.

2. Robert E. Dinnebier and Simon J. L. Billinge, Editor, **Powder diffraction: theory and practice**, Royal Society of Chemistry, London England, 2008.

3. Moneeb T. M. Shatnawi, Christopher L. Farrow, Ping Chen, Punit Boolchand, Asel Sartbaeva, M. F. Thorpe and Simon J. L. Billinge, **Search for a structural response to the intermediate phase in Ge_xSe_{1-x}glasses**, *Phys. Rev. B* **77**, 94134 (2008).

4. S. J. L. Billinge and I. Levin, **The problem with determining atomic structure at the nanoscale**, *Science* **316**, 561-565 (2007).

5. F. Inam, Moneeb T. Shatnawi, D. Tafen, S. J. L. Billinge, P. Chen and D. A. Drabold, **An intermediate phase in Ge_xSe_{1-x} glasses: experiment and simulation**, *J. Phys: Condens. Mat.* **19**, 455206 (2007).

6. Hasan Yavas, E. Ercan Alp, Harald Sinn, Ahmet Alatas, Ayman Said, Yuri Shvyd'ko, Thomas Toellner, Ruben Khachatryan, Simon J. L. Billinge, M. Zahid Hasan and Wolfgang Sturhahn, **Sapphire analyzers for high-resolution x-ray spectroscopy**, *Nucl. Instrum. Methods A* **582**, 149-151 (2007).

7. S. J. L. Billinge, **Nanostructure studied using the atomic pair distribution function**, *Z. Kristallogr. Suppl.* **26**, 17-26 (2007).

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9. S. J. L. Billinge, **Structure Determination and Phase Analysis using Neutron Diffraction**, *JOM-J. Min. Met. Mat. S.* **58**, 47-51 (2006).

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11. David Cherba, William Punch, Phil Duxbury, Simon J. L. Billinge and Pavol Juhás, **Conformation of an Ideal Bucky Ball Molecule by Genetic Algorithm and Geometric Constraint from Pair Distance Data**, In **GECCO-2005 Genetic and Evolutionary Computation Conference Proceedings**, (, New York, 2005), , Eds., pp. .

12. S. Brühne, E. Uhrig, K.-D. Luther, W. Assmus, M. Brunelli, A. S. Masadeh and S. J. L. Billinge, **PDF from X-ray powder diffraction for nanometer-scale atomic structure analysis of quasicrystalline alloys**, *Z. Kristallogr.* **220**, 962-967 (2005).

13. S. Brühne, E. Uhrig, C. Gross, W. Assmus, A. S. Masadeh and S. J. L. Billinge, **The local atomic quasicrystal structure of the icosahedral $Mg_{25}Y_{11}Zn_{64}$ alloy**, *J. Phys: Condens. Mat.* **17**, 1561-1572 (2005).

14. Chupas P. J., Chaudhuri S., Hanson J. C., Qiu X., Lee P. L., Shastri S. D., Billinge S. J. L. and Grey C. P., **Probing local and long-range structure simultaneously: an in-situ study of the high-temperature phase transition of \alpha-AlF_3**, *J. Am. Chem. Soc.* **126**, 4756-4757 (2004).

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16. S. J. L. Billinge and M. G. Kanatzidis, **Beyond crystallography: the study of disorder nanocrystallinity and crystallographically challenged materials**, *Chem. Commun.* **7**, 749-760 (2004).

17. Xiangyun Qiu, Emil S. Bozin, Pavol Juhás, Thomas Proffen and Simon J. L. Billinge, **Reciprocal space instrumental effects on the real space neutron atomic pair distribution function**, *J. Appl. Crystallogr.***37**, 110-116 (2004).

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19. B. H. Toby and S. J. L. Billinge, **Determination of standard uncertainties in fits to pair distribution functions**, *Acta Crystallogr. A* **60**, 315-317 (2004).

20. E. S. Bozin, V. Petkov, P. W. Barnes, P. M. Woodward, T. Vogt, S. D. Mahanti and S. J. L. Billinge, **Temperature dependent total scattering structural study of $CaCu_3Ti_4O_{12}$**, *J. Phys: Condens. Mat.* **16**, S5091-S5102 (2004).

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28. S. J. L. Billinge, **Complex materials: beyond crystallography**, *Z. Kristallogr.* **217**, 282 invited contribution (2002).

29. V. Petkov, S. J. L. Billinge, T. Vogt, A. S. Ichimura and J. L. Dye, **Structure of intercalated Cs in zeolite ITQ-4: an array of metal ions and electrons confined in a pseudo-1D nanoporous host**, *Phys. Rev. Lett.* **89**, 075502 (Highlighted in Phys. Rev. Focus: http://focus.aps.org/story/v10/st4) (2002).

30. Th. Proffen, V. Petkov, S. J. L. Billinge and T. Vogt, **Chemical short range order obtained from the atomic pair distribution function**, *Z. Kristallogr.* **217**, 47 (2002).

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