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The objective is to improve thermal expansion, specific heat, molar volume, and bulk moduli predictions at the highest temperatures and pressures. In those regions experiments are difficult and data is often marginally reliable. In a series of papers, we have developed models for predicting these properties for a wide range of metals, ceramics and semiconductors. By considering the influence of thermal defects on thermal expansion it has been possible to provide a quantitative relationship for thermal expansion and molar volume from near absolute zero to the melting point for refractory metals aluminum and copper. Over the course of the project we have combined our improved properties with finite element methods to calculate residual stresses important for the fabrication and reliability of group III-V Nitride devices and tungsten carbide.

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Thermophysical Properties and Phase Equilibria of Materials Systems

R.R. Reeber, D.Brenner, K.Wang and John Prater

The objective is to improve thermal expansion, specific heat, molar volume, and bulk moduli predictions at the highest temperatures and pressures. In those regions experiments are difficult and data is often marginally reliable. In a series of papers, we have developed models for predicting these properties. By considering the influence of thermal defects on thermal expansion it has been possible to provide quantitative relationships for thermal expansion and molar volume from near absolute zero to the melting point for a wide range of oxides, carbides, and metals. Over the course of the project we have combined our improved properties with finite element methods to calculate residual stresses important for the fabrication and reliability of group II-V Nitride devices and cutting tool materials such as tungsten carbide. We provided quantitative expressions for the thermal expansion of important cubic and hexagonal semiconductors (nitrides, phosphides, arsenides etc.) from cryogenic temperatures (approaching 0^{o}K) to near their melting points. A list of publications and presentations follows.

Publications supported by ARO under DAAH04-93-D-0003.

1. Wang, K. and R. R. Reeber, High temperature bulk moduli and self-diffusion for tantalum and tungsten, *High Temperature and Materials Science,* **36**, 37-45, 1996.

2. Reeber, R. R. and K. Wang, High temperature/pressure thermal expansion of elemental semiconductors and tungsten, *Proceedings of The 20th Army Science Conference,* Norfolk, VA, (June, 1996)

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5. Wang, K. and R. R. Reeber, Thermal expansion of copper, *High Temperature Materials Science,* **35,** 181-186, 1996.

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9. Wang, K. and R. R. Reeber, High temperature thermal property prediction for MgO,KCl and ZnS, in *Computer-Aided Design of High Temperature Materials,* Edited by A. Pechenik, R. K. Kalia, and P. Vashishta, Oxford University Press, New York, 1999, pp. 473-482.

10. Wang, K. and R. R. Reeber, Thermal residual stress modeling in AlN and GaN multilayer samples,*MRS Internet J. Nitride Semicond.,* **Vol. 4S1**, G3.18, 1999 http://nsr.mij.mrs.org/4S1/G3.18/).

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13. Wang, K. and R. R. Reeber, Mode Grüneisen parameters and negative thermal expansion of ZrW_2O_8 and $ZrMo_2O_8$, *Applied Physics Letters*, **76(16)**, 2203-2204, 2000.

14. Wang, K. and R. R. Reeber, The perfect crystal, thermal vacancies and the thermal expansion of aluminium, *Philosophical Magazine A*, **80(7)**, 1629-1643, 2000.

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16. Wang, K, RR Reeber and Salama, K "Fourth-order elastic constants of magnesium oxide" PHYSICA STATUS SOLIDI B-BASIC RESEARCH, **228** pp.837-845 (2001).

17. Wang, K and RR Reeber "Thermal expansion and elastic properties of InN" APPLIED PHYSICS LETTERS, **79**, (11) pp 1602-1604, (2001).

18. Reeber, RR and K. Wang "High temperature elastic constant prediction of some group III-nitrides" MRS INTERNET JOURNAL OF NITRIDE SEMICONDUCTOR RESEARCH **6**, p1-5, (2001).

Conference Talks:

1. Wang, K. and R. R. Reeber, Thermoelastic Properties of Group IIA Oxides, The American Ceramic Society 103rd Annual Meeting, Indianapolis, IN, Apr. 22-25, 2001
2. Wang, K., W. M. Ashmawi, M. A. Zikry, R. R. Reeber, Deformation and failure modes of thin film layered systems, MRS Fall Meeting, Boston, MA, Nov.27-Dec.1, 2000.
3. Reeber, R. R. and K. Wang, High temperature elastic constant prediction of some Group III-Nitrides, MRS Fall Meeting, Boston, MA, Nov.27-Dec.1, 2000.
4. Wang, K. and R. R. Reeber, High temperature/pressure thermophysical properties prediction, *MRS Spring Meeting*, San Francisco, CA, Apr. 24-28, 2000.
5. Ashmawi, W. M., K. Wang, R. R. Reeber, M. A. Zikry, Design guidelines for thin film layered systems, *MRS Spring Meeting*, San Francisco, CA, Apr. 24-28, 2000.
6. R. R. Reeber and K. Wang, Thermal expansion and lattice parameters of important semiconductors and substrates, *MRS Spring Meeting*, San Francisco, CA, Apr. 24-28, 2000.
7. Wang, K. and R. R. Reeber, Mode Grüneisen parameters and negative thermal expansion of zirconium tungstate, 51st Pacific Coast Regional Basic Science Division and Electronic Division Meeting of The American Ceramic Society, Bellevue, Washington, Oct. 27-29, 1999.
8. Wang, K and Robert R. Reeber, "High temperature/pressure thermophysical property prediction", Vanderbilt University-ARO Workshop on "Rapid Manufacturing/The Factory After-Next", Nashville, TN, Dec.13-16, 1998.
9. Wang, K. and R. R. Reeber, Thermal residual stress modeling in AlN and GaN multilayer samples, *MRS Fall Meeting*, Boston, Nov. 30 - Dec. 4, 1998.
10. Wang, K. and R. R. Reeber, Finite element modeling of thermal residual stress in Tungsten/Tungsten-Carbide composites, *The 22nd Annual Cocoa Beach Conference and Exposition On Composites, Advanced Ceramics, Materials and Structures*, The American Ceramic Society, Cocoa Beach, FL, Jan. 20-24, 1998.
11. Wang, K. and R. R. Reeber, Thermal properties of AlN and GaN, *MRS Fall Meeting*, Boston, Dec. 1-5, 1997.
12. Wang, K. and R. R. Reeber, High temperature/pressure thermal expansion of tungsten carbide, *The American Ceramic Society's 99th Annual Meeting*, Cincinnati, May 4-7, 1997.
13. Wang, K. and R. R. Reeber, High temperature thermal property prediction for MgO, KCl and ZnS, *Conference on Computer-Aided Design of High-Temperature Materials*, Santa Fe, NM, July 30 - August 2, 1997.
14. Wang, K. and R. R. Reeber, High temperature thermal expansion, bulk moduli and self-diffusion for tantalum and tungsten, *Army Research Office-University of Michigan Workshop on Hot Gas Erosion and Wear of Materials*, Ann Arbor, Michigan, September, 1996.
15. Reeber, R. R. and K. Wang, High temperature/pressure expansion of elemental semiconductors and tungsten, *20th Army Science Conference, Norfolk, Virginia*, June, 1996
16. Reeber, R.R. and K. Wang, Lattice parameters and thermal expansion of 6-H SiC, *The American Ceramic Society Annual meeting* April 2002, St. Louis, Mo.

Work completed in 2002.

The work of thermoelastic properties of Group IIA oxides at high temperature/pressure is almost finished and is in the process of being written up for journal publication. The thermal expansion at high temperatures was estimated and predicted with our earlier model. The elastic constants of these oxides have been predicted by a corresponding relationship where directional characteristic temperature model was utilized. Excellent agreement with available data was obtained.

The work on lattice parameter and thermal expansion of SiC has been completed. The data processing of neutron powder diffraction experiments at the NIST National reactor facility is finished. The interpretation of our low temperature experimental data with other author's results in high temperatures and the results were presented as an invited paper at the April 2002 Ceramic Society Annual Meeting in St. Louis,Mo.

List of personnel supported on the project:

Mr. W. Ashmawi, Mechanical Engineering graduate student
Dr. Kai Wang, Adjunct Assistant Professor
Dr. Robert Reeber Adjunct Research Professor
Dr. Donald Brenner,Associate Professor

Report of inventions:
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