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PERSONAL DETAILS

Date of birth: 01-01-1962
Marital status: Married (with three children)
Nationality: Australian

EDUCATION

Ph.D. degree in Physics in 1998	Curtin University of Technology, Perth, Australia
M.Sc. degree in Physics in 1991	Curtin University of Technology, Perth, Australia
PostGradDip degree in Physics in 1989	Curtin University of Technology, Perth, Australia

PROFESSIONAL EXPERIENCE

2005-present	COMPRES Research Fellow, Virginia Polytechnic Institute & State University
2004-2005	Research Associate, University of British Columbia
2002-2004	Research Fellow, Institut Laue Langevin (ILL) Neutrons for Science
2000-2002	Research Scientist, Ruhr Universitaet Bochum
1998-2000	Postdoctoral Fellow, NIST & State University of New York at Stony Brook
1994-1998	Tutor of Physics, Curtin University of Technology
1986-1994	Lecturer of Physics & Head of Physics Laboratory, Indonesian Institute of Technology

HONORS AND AWARDS

- Invited speaker to LANSCE User Group (LUG-7) Meeting, Los Alamos, 2005
- Invited speaker to high intensity pressure preferred orientation (HIPPO) workshop, Santa Fe, 2001
- Elected member of the International Center for Diffraction Data, 1998
- Curtin University of Postgraduate Research Scholarship, an ALCOA Australia Limited supplementary scholarship and a de Laeter Trust Fund supplementary scholarship, 1994-1998
- Elected member of the Australian X-ray Analytical Association, 1988
- Elected member of the Indonesian Physical Society, 1980
- Ted Maslen Scholarship, 1997
- IUCr Young Scientist Scholarship, 1991
- Elected member of the Society of Crystallographers in Australia and New Zealand, 1989
- International Development Program of Australian Universities Scholarship, 1987-1991
- The 11th of March Decree Letter Scholarship, 1980-1986

PROFESSIONAL SOCIETIES

- International Center for Diffraction Data
- Society of Crystallographers in Australia and New Zealand
- Australian X-ray Analytical Association
- Indonesian Physical Society

RESEARCH AND SCHOLARLY ACTIVITIES

I am one of a small group of qualified crystallographers in Western Australia, having completed a PhD degree in Physics, majoring in applied crystallography at Curtin University of Technology. My research involves aspects of crystallographic texture, martensitic phase transformation and structure refinement in polycrystalline materials with the aim of understanding the relationship between atomic structure, microstructure and physical properties of materials. I have extensive experience in a number of areas - Rietveld refinement of polycrystalline structures using neutron and X-ray diffraction data, texture measurements with both neutrons and X-rays, and neutron strain scanning measurements of internal stresses in engineering materials. Comparative evaluation of the March model and generalized spherical harmonic texture models using X-ray Bragg-Brentano diffractometry for uniaxially-pressed molybdenite and calcite powders has been continuously conducted. Parallel neutron diffraction data of uniaxially-pressed molybdenite and calcite powders and also the technologically important polycrystalline *nickel-titanium* shape memory alloy were measured using worldwide neutron facilities at ANSTO, GKSS, HMI, ILL, LANSCE and NIST, in order to compare the bulk, or global, texture and strain information with near-surface characterizations obtained by X-rays (Sitepu *et al.* (2005). *Journal of Applied Crystallography*, **38**, 158-167).

I have used the third generation synchrotron X-ray source at the European Synchrotron Research Facility in Grenoble to determine the crystal structure of the R-phase in $\text{Ti}_{50.75}\cdot\text{Ni}_{47.75}\cdot\text{Fe}_{1.50}$ alloy. Combined refinements using both the neutron and synchrotron diffraction data sets were carried out using the $P\bar{3}$, $P3$ and $P31m$ space groups. For all three of these models the agreement between observed and calculated curves is excellent, although only the refinement in space group $P\bar{3}$ converges. Large shifts on the atomic positions remain after many cycles of refinement in space groups $P31m$ and $P3$, indicating that our data were not sufficient to determine these parameters. Comparing the three models shows that $P\bar{3}$ only contains 6 atom parameters, compared to 17 for $P3$ and 11 for $P31m$. Given that the refinements would only converge using space group $P\bar{3}$ and that no significant improvement in fit is found for the other space groups, we conclude that this space group with only six degrees of freedom in the atomic positions is sufficient to describe our data. Comparison of the Rietveld fit shows that the peak intensities are quite different in the neutron and synchrotron data sets. This is due to the negative scattering length for Ti, so that by exploiting combined neutron and X-ray refinements there is excellent discrepancy between the two atomic sites. Trial refinements initially using only the synchrotron data sometimes found a false minimum with somewhat worse *goodness of-fit* indices, however, when both data sets were used the same minimum was always recovered (Sitepu (2003). *Textures and Microstructures*, **35**, 185-195; Sitepu *et al.* (2005). *Mat. Sci. Forum*, **495-497**, 255-260).

Also, I have used the third generation synchrotron X-ray source at the Advanced Photon Source (APS) in Argonne to develop semi-quantitative analytical tools for non-destructive in-situ identification and characterization of mineral inclusions in diamonds. The data were collected at the Pacific Northwest Consortium (PNC-CAT) 20-ID microprobe beamline and yielded the first high-resolution maps of Ti, Cr, Fe, Ni, Cu, and Zn for natural diamond grains, along with quantitative synchrotron micro-X-ray Fluorescence (μSXRF) of select chemical elements in exposed kimberlite indicator mineral grains. The results indicated that (i) the distribution of diamond inclusions inside the natural diamond host, both visible and invisible using optical transmitted-light microscopy can be mapped with synchrotron μXRF analysis, (ii) the relative abundances of chemical elements determined by μSXRF elemental analyses are broadly similar to their expected ratios in the mineral and therefore can be used to identify inclusions in diamonds in situ and (iii) synchrotron μXRF quantitative analysis provides accurate estimates of Cr contents of exposed polished minerals when calibrated using the concentration of Fe as a standard. Corresponding Cr K-edge results obtained from synchrotron micro-X-ray Absorption Near Edge Structure (μXANES) analyses on selected inclusions yielded unique information regarding the formal oxidation state and local coordination of Cr (Sitepu *et al.* (2005). *American Mineralogist*. In Press).

The objectives of my recent research are (i) to explore the changes in the crystal structures of calcite I, II and III at high pressures and temperatures and to resolve the crystal structure of calcite III; (ii) to determine the pressure and temperature boundaries between calcite I, II and III. The single crystal X-ray diffraction at high pressure and neutron high pressures and temperatures results from this study will be presented to the earth science community through COMPRES as part of an initiative to inform the earth science community about the potential of *in situ* high-pressure, high-temperature neutron diffraction studies that determine structure, texture and strain (<http://www.crystal.vt.edu/compres/> and (<http://www.compres.stonybrook.edu/Newsletter>). Also, the results will be published at the referred journals.

RESEARCH PUBLICATIONS

1. **H. Sitepu**, M.G. Kopylopa, D.H. Quirt, J.N. Cutler and T.G. Kotzer. (2005). *Synchrotron micro-X-ray fluorescence maps of natural diamonds: First steps in identification of mineral inclusions in-situ*. American Mineralogist. In Press.
2. **H. Sitepu**, J.P Wright, T. Hansen, D. Chateigner, H.-G. Brokmeier, C. Ritter and T. Ohba. (2005). *Combined synchrotron and neutron structural refinement of R-phase in $Ti_{50.75}Ni_{47.75}Fe_{1.50}$ shape memory alloy*. Materials Science Forum. **495-497**, 255-260.
3. **H. Sitepu**, B.H. O'Connor and D.Y. Li. (2005). *Comparative evaluation of the March and generalized spherical harmonic preferred orientation models using X-ray diffraction data for molybdenite and calcite powders*. Journal of Applied Crystallography. **38**, 158-167.
4. **H. Sitepu**, H.G. Brokmeier, D. Chateigner and J.P. Wright. (2005). *Crystallographic phase composition and structural analysis of Ti-Ni-Fe shape memory alloy by synchrotron diffraction*. Solid State Phenomena. **105**, 139-144.
5. **H. Sitepu** and H.G. Brokmeier. (2005). *Use of neutron diffraction for describing texture of isostatically-pressed molybdenite powders*. Solid State Phenomena. **495-497**, 83-88.
6. **H. Sitepu**, B.H. O'Connor and D.Y. Li. (2004). *Deriving the Bulk modulus of a single-phase powder from March preferred orientation parameter*. Physica B: Condensed Matter, **350**, E577-E580.
7. J. Khalil-Allafi, W. W. Schmahl, M. Wagner, **H. Sitepu**, D. M. Toebbens and G. Eggeler. (2004). *The influence of temperature on lattice parameters of coexisting phases in NiTi shape memory alloys - a neutron diffraction study*. Materials Science and Engineering A, **378**, 161-164.
8. **H. Sitepu**, and H.G. Brockmeier. (2004). *Quantitative texture analysis and phase fraction of nickel-titanium shape memory alloys by means of neutron diffraction*. Materials Science Forum, **443-444**, 267-270.
9. D. J. Hughes, P. J. Webster, B. Malard, N. Ratel, **H. Sitepu** and A. Dale (2004). *FaME38: a new approach to materials engineering at the ILL-ESRF*, Physica B: Condensed Matter, **350**, 110-112
10. **H. Sitepu**, B.H. O'Connor, H.-G. Brockmeier, A. Benmarouane, T. Hansen and C. Ritter. (2004). *Texture correction in neutron powder diffraction data of molybdenite using the generalized spherical harmonic model*. Physica B: Condensed Matter, **350**, E573-E576
11. **H. Sitepu** (2003). *Use of synchrotron diffraction data for describing crystal structure and crystallographic phase analysis of R-phase NiTi shape memory alloy*. Textures and Microstructures, **35**, 185-195.
12. **H. Sitepu**, W. W.Schmahl, M. Kloenne, W. Predki and T. Pirling. (2003). *Measurements of strain, texture and phase fraction in aged Ni-rich NiTi shape memory alloy by neutron diffraction technique under in situ torsional loading*. Journal of de Physique IV, **112**, 811-814.
13. P.J. Webster, D.J. Hughes, **H. Sitepu**, B. Malard, N. Ratel and A.M. Dale. (2003). *FaME38: A new approach to materials science at the ILL-ESRF*. Journal of Neutron Research. **11**, 263-266.
14. **H. Sitepu**, W. W.Schmahl and T. Reinecke, J. Khalil Allafi and G. Eggeler. (2003). *Phase fractions of B2, B19', R-phase and Ni_4Ti_3 in NiTi alloys during two-step transformations*. Journal of de Physique IV, **112**, 677-680.
15. **H. Sitepu**, W.W. Schmahl, G. Eggeler, J. Khalil Allafi, and D.M. Többens. (2003). *A neutron diffraction study of the martensitic transformation in aged Ni-rich NiTi Alloys*. Journal of de Physique IV, **112**, 643-646.
16. **H. Sitepu**. (2002). *Assessment of preferred orientation with neutron powder diffraction data*. Journal of Applied Crystallography, **35**, 274-277.

17. **H. Sitepu**, W.W. Schmahl, J. Khalil Allafi, G. Eggeler, A. Dlouhy, D.M. Tobbens and M. Tovar. (2002). *Neutron diffraction phase analysis during thermal cycling of a Ni-rich NiTi shape memory alloy using the Rietveld method*. Scripta Materialia, **46**, 543-548.
18. **H. Sitepu**, W.W. Schmahl and R.B. Von Dreele. (2002). *Use of Rietveld refinement with the generalized spherical-harmonic model for describing crystallographic texture in polycrystalline NiTi shape memory alloys with time-of-flight neutron powder diffraction data*. Applied Physics. **A74**, S1676-S1678.
19. **H. Sitepu**, W.W. Schmahl, J. Khalil Allafi, G. Eggeler, T. Reinecke, H.G. Brockmeier, M. Tovar and D.M. Töbrens. (2002). *A quantitative analysis of martensitic phases and their crystallographic texture in an aged Ni-rich NiTi alloy using X-ray and neutron diffraction data*. Materials Science Forum, **Vol. 394-395**, 237-240.
20. **H. Sitepu**, W. W.Schmahl and J. K.Stalick. (2002). *Correction of intensities for preferred orientation in neutron powder diffraction data of NiTi shape memory alloy using the generalized spherical-harmonic description*. Applied Physics. **A74**, S1719-S1721
21. **H. Sitepu**, W.W. Schmahl and R.B. Von Dreele. (2002). *Quantitative texture analysis in polycrystalline shape memory alloys NiTi neutron diffraction data by Rietveld refinement with the generalized spherical-harmonic description*. Materials Science Forum, **Vol. 394-395**, 233-236.
22. **H. Sitepu**, J.K. Stalick, H.J. Prask, M.D. Vaudin and S. Sampath. (2002). *Crystallographic preferred orientation and phase fraction of plasma spray coatings by means of neutron and X-ray diffraction*. Physics Journal of the Indonesian Physical Society, **A5 0212**, 1-10.
23. M. Kaack, T. Yohannes, J. Gibkes, J. Pelzl, A. Heckmann, **H. Sitepu**, W.W. Schmahl, N. Tankovsky. (2002). *Elastic bulk and surface properties of thermally and mechanically cycled NiTi shape memory alloys*. Materials Science Forum. **Vol. 394-395**, 341-344.
24. **H. Sitepu**, H.J. Prask and M.D. Vaudin. (2001). *Texture characterization in X-ray and neutron powder diffraction data using the generalized spherical-harmonic*. Advances in X-ray Analysis, **44**, 241-246.
25. **H. Sitepu**, B.H. O'Connor and D.Y. Li. (1997). *Preferred orientation in powders and its influence on Rietveld X-ray powder diffraction pattern-fitting*. Indonesian Journal of Physics, **1**, 73-98.
26. **H. Sitepu**, B.H. O'Connor and D.Y. Li. (1992). *Texture characterization in X-ray powder diffraction using the March formula*. Advances in X-ray Analysis, **35**, 277-283.
27. B.H. O'Connor, D.Y. Li and **H. Sitepu**. (1991). *Strategies for preferred orientation corrections in X-ray powder diffraction using line intensity ratios*. Advances in X-ray Analysis, **34**, 409-415.