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Collaborative Research: Multiscale Analysis of Geological Structures That Influence Crustal Seismic Anisotropy

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Cover

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Signature of Submitting Official (signature shall be submitted in accordance with agency specific instructions)	Senthil Vel

Accomplishments

* What are the major goals of the project?

The major goals of this 2-year collaborative project were to develop a rigorous and integrated methodology for studying

crustal material anisotropy at different scales and to analyze their combined effects on seismic wave propagation. The primary focus of the research was on (a) macroscale structural geometries and their influence on the seismic response of rock fabrics and (b) the influence of microstructural features and textures on seismic anisotropy.

*** What was accomplished under these goals (you must provide information for at least one of the 4 categories below)?**

Major Activities:

I) The influence of microstructure on the seismic anisotropy of rocks

We have worked on the characterization of bulk elastic properties and seismic anisotropy of crustal rocks. The bulk elastic properties and corresponding wave velocities were calculated for synthetic rock samples with varying amounts of muscovite and quartz, different muscovite and quartz grain orientations and varying spatial distributions of the muscovite grains to investigate the sensitivity of seismic wave speed anisotropy on these characteristics. The asymptotic expansion homogenization method combined with finite element modelling was used to calculate bulk stiffness tensors for representative rock volumes and the wave velocities were obtained from these tensors using the Christoffel equation. The aim of this task was to (a) demonstrate how wave speeds computed from the rigorous asymptotic expansion homogenization method compare with those generated using stiffness tensors derived from commonly applied analytic estimates, and (b) explore how different microstructural variables influence seismic wave speeds.

II) The influence of crenulation cleavage development on the bulk elastic properties and seismic wave velocities of phyllosilicate-rich rocks.

In addition to mineralogy, the textures found in rocks influence the way seismic waves travel through them. Phyllosilicates are elastically highly anisotropic and are therefore thought to be an important contributor to seismic anisotropy in the crust. Crenulation cleavage is the most commonly found texture in multiply-deformed, phyllosilicate-rich crustal rocks. We calculated the bulk elastic properties and resulting wave velocities for three rock samples that preserved different stages of crenulation cleavage: a planar foliation, a moderately developed crenulation cleavage, and a well-developed crenulation cleavage. Mineral orientation maps were obtained using electron backscatter diffraction (EBSD) and calculations were made using asymptotic expansion homogenization combined with the finite element method.

III) Seismic anisotropy of folded structures

Many volumes of interest in the continental crust are non-uniform as a result of compositional variations, metamorphic gradients or deformational features such as folds and shear zones. Non-uniform anisotropic materials can be represented as a bulk effective medium obtained by volumetric averaging of the corresponding stiffnesses. We have developed a tensorial approach to quantify the effects of structure on rock anisotropy. If the rocks within a structure are fairly uniform or the seismic scale of interest allows for averaging of smaller scale heterogeneity, the original rock within the structure can be simplified into a representative rock of stiffness that fills the structure. In such cases, tensor averaging methods permit the decomposition of the effective media stiffness into the product of a structural geometry operator (SGO) and the representative rock stiffnesses. The SGO can be analytically or numerically computed if a structure of interest can be described mathematically. We have obtained the SGOs for common fold geometries such as sinusoidal, chevron, box and cusped, which can be used to transform the original rock stiffness into a geological effective medium for seismic studies. We have analyzed the influence of fold type and limb angle on seismic wave speeds and

seismic anisotropy in three dimensions. We have compared our models of the anticipated wave propagation through the folds with synthetic seismograms in order to validate our approach and explore how real seismic observables can provide information on the geometry and kinematics of in situ crustal deformation.

IV) Development of a toolbox for the analysis of EBSD data

A Matlab-based Graphical User Interface (GUI) program has been developed for the analysis of real and synthetic polycrystalline rock microstructures. The GUI is capable of importing EBSD information for a rock sample and determining the corresponding effective properties, including elastic stiffnesses, wave speeds, and anisotropies using asymptotic expansion homogenization method. The beta version of the open-source software is currently being tested by several EBSD labs. It is currently available for download through the following web site:

http://umaine.edu/mecheng/faculty-and-staff/senthil-vel/software/ESP_Toolbox/.

Future developments will allow for stress analyses of the imported microstructures as well as the simulation of fracture propagation.

Specific Objectives: The major findings of our research are as follows,

Significant Results: I) The influence of microstructure on the seismic anisotropy of rocks

Our results show that the muscovite grain orientations have a significant influence on the wave speeds. Increasing the modal fraction and alignment of muscovite grains leads to greater seismic anisotropy of the rock. The P-wave speed at an incidence angle of 45 degrees between the foliation and seismic wave path is dependent on all tested microstructural variables, with the orientation distribution of muscovite grains having the largest effect. Although we have explicitly considered only muscovite grains in this study, the methodology and observations are expected to apply in general to other phyllosilicates.

II) The influence of crenulation cleavage development on the bulk elastic properties and seismic wave velocities of phyllosilicate-rich rocks.

The seismic anisotropies calculated using the commonly used Voigt-Reuss-Hill average deviate up to 19.4% from the values calculated using asymptotic expansion homogenization. Rocks that are characterized by the planar foliation and the moderately developed crenulation cleavage are highly anisotropic, with anisotropies up to 34.2%, whereas the rock characterized by the well developed crenulation cleavage are only mildly isotropic, with a P-wave anisotropy of 15.5% and S-wave anisotropy of 10.7%. Progressive development of the fabric also causes the orientations of P- and S-wave velocity maxima, and S-wave polarization directions, to change markedly. Despite the high anisotropy imparted by a planar schistosity, the variety of folds and fabrics typically found in phyllosilicate-rich rocks within larger-scale crustal volumes will tend to mute the anisotropy, possibly to the point of appearing nearly isotropic.

III) Effect of fold structures on seismic anisotropy in continental crust

The concept of structural geometry operator enables the algebraic separation of the effects of the fold geometry from the local rock stiffnesses and allows for the direct investigation of structural geometry effects on the bulk elastic stiffnesses and seismic wave speeds. The synthetic seismograms are in good agreement with anticipated wave propagation for our hypothetical folds. Thus, it might be possible to identify hinge shape, limb angle, and even orientation of subsurface folds in the

crust using seismic signals from natural sources detected by appropriate novel array deployments and comparing with our models, and in turn obtain information on the kinematics of in situ crustal deformation.

Key outcomes or
Other achievements:

The major achievements of the project are as follows:

(a) The concept of seismic effective media (EMs) was used to represent earth volumes through which seismic waves travel. An important contribution of this project was the separation of the influence of structural geometry from the representative rock stiffness using the concept of a structural geometry operator (SGO). We have developed SGOs for different fold geometries, such as sinusoidal, chevron, parabolic, box and cusped folds. They can be used to calculate the seismic velocities and anisotropies of common fold geometries.

(b) A comprehensive software package with a user-friendly graphical user interface has been developed for the calculation of bulk elastic properties and seismic wave speed from EBSD-derived rock data based on rigorous micromechanics.

* What opportunities for training and professional development has the project provided?

The four Ph.D. students who worked on this project (Felice Naus-Thijssen, Won Joon Song, Alden Cook and Jacob Pelletier) were provided rich opportunities for learning both analytical methods via the SEM/EBSD system, and numerical/computational methods using finite elements and Matlab-based GUI development.

* How have the results been disseminated to communities of interest?

We have sent a beta version of the GUI software developed as a part of this research effort to several EBSD labs for testing. Once we hear back from them and the appropriate modifications have been made, we will make the software and source code freely available to the public through the following web site: http://umaine.edu/mecheng/faculty-and-staff/senthil-vel/software/ESP_Toolbox/.

Major research findings have been disseminated through refereed journal papers and conference presentation.

Products

Books

Book Chapters

Conference Papers and Presentations

Naus-Thijssen, F.M.J., Goupee, A.J., Johnson, S.E., Vel, S.S. (2009). *Computational modeling of rock fabrics: Implications for seismic anisotropy in the Crust*. American Geophysical Union, Fall Meeting. San Francisco, California. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Song, W.J., Vel, S.S., Johnson, S.E., Okaya, D. (2012). *Effect of fold structures on seismic anisotropy in continental crust*. European Geological Union General Assembly. Vienna, Austria. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Johnson, S.E., Vel, S.S., Gerbi, C.C., Cook, A.C., Song W.J., Okaya D. (2011). *Evaluating the effects of shear zone development on seismic anisotropy in the deep cratonic crust: natural examples and computational methods*. Geological Society of America Annual Meeting. Minneapolis, MN. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Okaya, D., Johnson, S.E., Vel, S.S., Christensen, N.I. (2011). *Factors for the use of seismic anisotropy to examine crustal deformation and metamorphism within cratons*. Geological Society of America Annual Meeting. Minneapolis,

MN. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Vel, S.S., Johnson, S.E., Cook, A.C., Goupee, A.J., Song, W.J., Okaya, D. (2011). *Integrated analytical-computational framework for the calculation of bulk elastic properties and seismic wave speeds in polycrystalline materials*. Geological Society of America Annual Meeting. Minneapolis, MN. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Johnson, S.E., Naus-Thijssen, F.M.J., Vel, S.S., Goupee, A.J., Okaya, D.A. (2011). *Microscale Stress and Strain Distributions, Fabric Evolution, and Crustal Seismic Anisotropy*. Conference on the interrelationships between deformation and metamorphism, International meeting in honor of Tim Bell. Granada, Spain. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Johnson, S.E., Naus-Thijssen, F.M.J., Vel, S.S., Goupee, A.J., Okaya, D. (2009). *Numerical modeling of microstructural processes and fabric evolution: an essential step in exploring crustal seismic anisotropy*. Pardee Symposium on Crustal Tectonic Deformation as Revealed by Seismic Anisotropy, Geological Society of America Annual Meeting. Portland, Oregon. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Johnson, S.E., Vel, S.S., Gerbi, C.C., Song, W.J., Okaya, D.A., Cook, A. (2011). *The effects of strain localization and shear zone development on elastic anisotropy at a variety of scales*. Geological Society of America Penrose Conference. Cap de Creus, Catalonia, Spain. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Okaya, D., Johnson, S.E., Vel, S.S., Song, W.J., Christensen, N.I. (2012). *The role of length scales in bridging the gap between rock CPO and seismic signals of crustal anisotropy*. EGU General Assembly. Vienna, Austria. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Inventions

Nothing to report.

Journals

Naus-Thijssen, F.M.J., Goupee, A.J., Johnson, S.E., Vel, S.S., Gerbi, C. (2011). The influence of crenulation cleavage development on the bulk elastic and seismic properties of phyllosilicate-rich rocks. *Earth and Planetary Science Letters*. 311 212-224. Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Naus-Thijssen, F.M.J., Goupee, A.J., Vel, S.S., Johnson, S.E. (2011). The influence of microstructure on seismic wave speed anisotropy in the crust: Computational analysis of quartz muscovite rocks. *Geophysical Journal International*. 185 609-621. Status = PUBLISHED; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Okaya, D.A., Vel, S.S., Johnson, S., Song, W.J. (2013). The Modification of Crustal Seismic Anisotropy by Geological Structures ("Structural Geometry Anisotropy"). *Geochemistry Geophysics Geosystems*. . Status = UNDER_REVIEW; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Song, W.J., Vel, S.S., Johnson, S.E., Okaya, D.A. (2013). Effect of fold structures on seismic anisotropy in continental crust. *Geochemistry Geophysics Geosystems*. . Status = UNDER_REVIEW; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Vel, S.S., Cook, A.C., Johnson, S.E., Gerbi, C. (2013). A computational framework for the determination of bulk thermoelastic properties and microstress analysis of textured polycrystalline materials using SEM-EBSD data. *Computational Materials Science*. . Status = OTHER; Acknowledgment of Federal Support = Yes ; Peer Reviewed = Yes

Licenses

Nothing to report.

Other Products

Software or Netware.

Cook, A., Vel., S., Johnson, S.E., Gerbi, C., Song, W.J., 2013a. Elastic and Seismic Properties (ESP) Toolbox (beta version), http://umaine.edu/mecheng/faculty-and-staff/senthilvel/software/ESP_Toolbox/ . Open-source software for calculating the elastic and seismic properties of rocks using either EBSD data files or computer generated microstructures.

The GUI software is a standalone interface for the calculation of bulk elastic and seismic properties of heterogeneous and polycrystalline materials using image or EBSD data. The GUI includes a number of different homogenization techniques, including Voigt, Reuss, Hill, geometric mean, self-consistent and Asymptotic Expansion Homogenization (AEH) methods. The AEH method, which uses a finite element mesh, is more accurate than the other methods since it explicitly accounts for grain-scale elastic interactions. The user need only specify the microstructure and material properties of the individual minerals or phases. Once homogenization is performed, the bulk elastic stiffnesses and average density are used to compute seismic wave speeds and anisotropies. A post-processing interface allows the user to visualize seismic results as equal-area projections or contoured spheres. Results can be exported with publication quality in a number of different formats.

The GUI package is the result of a joint effort between the Mechanical Engineering Department (Alden Cook, Senthil Vel) and the School of Earth and Climate Sciences (Scott Johnson, Chris Gerbi and Won Joon Song) at the University of Maine. The coding was done in Matlab and C by Alden Cook.

Other Publications

Song, W.J., Cook, A., Gerbi, C., Vel., S., Johnson, S.E. (2013). *Elastic and Seismic Properties (ESP) Toolbox (beta version) Manual and Tutorial*. User's manual for our open-source software for calculating the elastic and seismic properties of rocks using EBSD data files or computer-generated microstructures. http://umaine.edu/mecheng/faculty-and-staff/senthil-vel/software/ESP_Toolbox/. Status = PUBLISHED; Acknowledgement of Federal Support = Yes

Patents

Nothing to report.

Technologies or Techniques

Nothing to report.

Thesis/Dissertations

Naus-Thijssen, F.M.J.. *Crenulation Cleavage Development and the Influence of Rock Microstructure on Crustal Seismic Anisotropy*. (2011). University of Maine. Acknowledgement of Federal Support = Yes

Websites

Microstructural Analysis of Bulk Elastic and Seismic Properties

http://umaine.edu/mecheng/faculty-and-staff/senthil-vel/software/ESP_Toolbox/

This is a site we developed for public access to our NSF-funded open-source software.

Participants/Organizations

What individuals have worked on the project?

Name	Most Senior Project Role	Nearest Person Month Worked
Vel, Senthil	PD/PI	2
Johnson, Scott	Co PD/PI	2
Cook, Alden	Graduate Student (research assistant)	6
Naus-Thijssen, Felice	Graduate Student (research assistant)	8

Pelletier, Jacob	Graduate Student (research assistant)	4
Song, Won Joon	Graduate Student (research assistant)	8

Full details of individuals who have worked on the project:

Senthil Vel**Email:** senthil.vel@maine.edu**Most Senior Project Role:** PD/PI**Nearest Person Month Worked:** 2**Contribution to the Project:** Theoretical and computational analysis of geological structures and rocks; advising graduate students.**Funding Support:** None**International Collaboration:** No**International Travel:** No

Scott E Johnson**Email:** johnsons@maine.edu**Most Senior Project Role:** Co PD/PI**Nearest Person Month Worked:** 2**Contribution to the Project:** Studied the influence of rock fabric on seismic anisotropy; EBSD analysis of rocks; advising graduate students.**Funding Support:** None**International Collaboration:** No**International Travel:** No

Alden Cook**Email:** Alden_Cook@umit.maine.edu**Most Senior Project Role:** Graduate Student (research assistant)**Nearest Person Month Worked:** 6**Contribution to the Project:** Development of a GUI toolbox for the analysis of EBSD data**Funding Support:** None**International Collaboration:** No**International Travel:** No

Felice Naus-Thijssen**Email:** Felice_Thijssen@umit.maine.edu**Most Senior Project Role:** Graduate Student (research assistant)**Nearest Person Month Worked:** 8**Contribution to the Project:** Investigated the influence of microstructure on the seismic anisotropy of rocks

Funding Support: None

International Collaboration: No

International Travel: No

Jacob Pelletier

Email: jacob.pelletier@gmail.com

Most Senior Project Role: Graduate Student (research assistant)

Nearest Person Month Worked: 4

Contribution to the Project: 3D analysis of polycrystalline rock microstructures

Funding Support: None

International Collaboration: No

International Travel: No

Won Joon Song

Email: wonjoon_song@umit.maine.edu

Most Senior Project Role: Graduate Student (research assistant)

Nearest Person Month Worked: 8

Contribution to the Project: Analysis of seismic anisotropy of folded structures

Funding Support: None

International Collaboration: No

International Travel: No

What other organizations have been involved as partners?

Name	Type of Partner Organization	Location
University of Southern California	Academic Institution	Los Angeles, CA

Full details of organizations that have been involved as partners:

University of Southern California

Organization Type: Academic Institution

Organization Location: Los Angeles, CA

Partner's Contribution to the Project:

Collaborative Research

More Detail on Partner and Contribution: Dr. David Okaya, Associate Research Professor of Earth Sciences investigated the propagation of seismic waves through folded structures using his 3D anisotropic finite difference wave propagation code.

What other collaborators or contacts have been involved?

NO

Impacts

What is the impact on the development of the principal discipline(s) of the project?

I) The graphical user interface and computational engine we have developed for calculating bulk elastic properties and seismic wave speed from EBSD-derived rock data will have an important impact on the geological and geophysical communities. The software is comprehensive, easy to use, and provides precise calculation owing to the use of asymptotic expansion homogenization methods as opposed to Voigt and Reuss approximations.

II) Structural Geometry Operators have been developed for common fold types. They will provide important insights into the seismic anisotropy of geological structures and make it easier to interpret seismic data.

What is the impact on other disciplines?

The computational tools we are developing are mainly for the Earth Sciences community, but are designed to be easily expanded for the Materials Science and Engineering communities. Given that we are an Earth Sciences/Engineering team, this extension into other disciplines is a natural result of our collaboration. The GUI software package developed for the analysis of EBSD-derived microstructures will also enable Materials Scientists to characterize the bulk properties and perform detailed stress analyses of engineered polycrystalline materials such as metallic alloys, ceramics and advanced composite materials.

What is the impact on the development of human resources?

Four PhD students were involved in this project, and they received excellent training in both Earth science and computational mechanics disciplines.

What is the impact on physical resources that form infrastructure?

This project funded a computer workstation for development and execution of our software products.

What is the impact on institutional resources that form infrastructure?

Nothing to report.

What is the impact on information resources that form infrastructure?

We are developing a suite of open-source software products that are available through a website that we created.

What is the impact on technology transfer?

Our open source software will be available to the commercial and private sectors and is likely to be well received by both.

What is the impact on society beyond science and technology?

Nothing to report.

Changes/Problems

Changes in approach and reason for change

Nothing to report.

Actual or Anticipated problems or delays and actions or plans to resolve them

Nothing to report.

Changes that have a significant impact on expenditures

Nothing to report.

Significant changes in use or care of human subjects

Nothing to report.

Significant changes in use or care of vertebrate animals

Nothing to report.

Significant changes in use or care of biohazards

Nothing to report.

Special Requirements**Responses to any special reporting requirements specified in the award terms and conditions, as well as any award specific reporting requirements.**

Nothing to report.