related glasses worldwide, in contrast with those from mid-ocean ridges or hot spots.

V32H-06 1715h

Origins of Newberry Volcano, Central Oregon: A Cascade Backarc, High Lava Plains, Basin and Range Shield Volcano?

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Newberry Volcano, located 60 km east of the central Oregon High Cascades resides in a complex tectonic and volcanic region. Understanding the petrogenesis of Newberry Volcano is important to understanding the regional geological framework because of its location at the confluence of the back-arc of the Oregon Cascades, the northern end of the Basin and Range, and the western end of the High Lava Plains (HLP). The latter province includes a NW trend of propagating rhyolitic volcanism whose youngest expression appears to be Newberry. A clear understanding of Newberry's relation to the Cascades is also important due to a scarcity of backarc volcanism in this region. The first goal of this study is to evaluate the range of composition of the primary magmas that make up the parent magma array for this system to evaluate the diversity of mantle materials involved and the degree of melting. This study uses major- and trace-element data from primitive basalts (> 8 wt % MgO, > Fo# 80) and melt inclusions, coupled with volatile elements (Cl, S, CO_2, and H_2O) from high-alumina olivine tholeiite (HAOT) lavas from Newberry Volcano, the HLP, the northern Basin and Range volcanics, and the Oregon Cascades in an attempt to evaluate the primitive compositions and melting dynamics at Newberry. Using this data we hope to discern Newberry's relative importance and relation to the surrounding volcanic regions. Preliminary melt inclusion data from Newberry and surrounding regions suggests that Newberry is slightly enriched in Ba (up to 750 ppm), K_2O (1 wt %), and Rb (24 ppm) relative to samples collected from the adjacent Basin and Range volcanics and the HLP. Also significant is that Nb and Ta are relatively depleted in the Newberry melt inclusions with K/Nb ranging from 600 to 1135 whereas the samples from the Basin and Range and HLP vary from 400-570 and 180-245, respectively. This, coupled with the Ba enrichment may suggest that a subduction-related fluid component is present in the mantle source region of Newberry magmas that is absent from the Basin and Range and HLP. Additionally, Cl concentrations in melt inclusions from several Newberry samples range from 200 to 1600 ppm, similar to values for primitive basalts in the High Cascades and much higher than values for magmas from the Basin and Range and HLP. The Cascades have been interpreted as a hot, dry arc and yet an apparent subduction-related fluid signature is observed as far as 300 km inland from the trench. Therefore, this data, while not conclusive, may have important ramifications for dehydration and fluid migration models beneath young, hot volcanic arcs.

V32H-07 1730h

Composite Chemostratigraphy of Lavas From the Casitas Shield, Descabezado Grande-Cerro Azul Volcanic Complex, Chilean Andes

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The Descabezado Grande-Cerro Azul (DGCA) volcanic complex is located at approximately 35.5 degrees S in the transitional Southern Volcanic Zone (SVZ) of the Chilean Andes. The complex is characterized by two large latest Pliocene to early Holocene volcanic edifices and many smaller vents rising above a plateau comprising lavas of an earlier shield-building stage, the Casitas Shield. This plateau has been deeply encised, revealing stacks of lava flows exposed along the valley walls. More than 100 lava flows from eight vertical stratigraphic sections have been analyzed for complete major and trace element abundances. These have been compiled in a composite chemical stratigraphy representing much of the history of this stage of volcanism. At least twelve eruptive episodes were identified based on field observations (soil development, erosional features, mingled top and bottom rubble zones, etc.). Lavas flowed south and west from the proposed vent location(s) primarily filling paleovalleys, constrained to the west by topographic highs composed of tilted metasediments and a granodioritic stock. A number of long flows served as the basis in the field for physical correlations between sections, and were used to evaluate within-flow compositional variation. The top flows on the shield have a single date of .34 My. The composite chemical stratigraphy shows changes in lava compositions reflecting both differences in parental magmas and the secular dominance of certain petrogenetic processes over others. In general, lavas become more evolved through episodes 1-5, and are relatively constant in composition during episodes 6-8. More mafic lavas erupted during episode 9, including lavas that are among the most primitive in the SVZ. These lavas are characterized by high Cr (254-267 ppm) and MgO (8-8.3%), and low LILE, P2O5, Al2O3, Na2O, and K2O, and probably represent a different parental magma. Lavas erupted during episodes 10 and 11 are progressively more evolved, becoming similar to lavas erupted more recently from Volcan Cerro Azul. Several cross-cutting basaltic dikes are characterized by high MgO (11.7%), Ni (226 ppm) and Cr (776 ppm) contents, and along with high-Sr lavas (972-1061 ppm) erupted during episode 3, extend the known compositional ranges for mafic lavas in the SVZ. Most of the compositional diversity occurs during periods of apparent low eruption rate with few lava flows, perhaps including some from separate short-lived vents. Periods of higher eruptive activity are characterized by less compositional range and flows often appear in the field with flow tops mingled with the bottom of the next flow. This composite chemical stratigraphy will be compared to one constructed at the nearby Tatara-San Pedro complex.

V32H-08 1745h

Volatile, Trace Element and Isotopic Variations of Mafic Arc Volcanic Rocks from Nicaragua and Costa Rica

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Quaternary volcanic rocks from the Central American Volcanic Arc in central Nicaragua and central Costa Rica exhibit major differences in their volatile, trace element and isotopic compositions. Olivine-hosted melt inclusions in Nicaraguan volcanic rocks with high Fo contents (>73) extend to high H_2O (up to 5.3%), S (10-6860 ppm) and Cl (490-2340 ppm) contents. The volcanic rocks have high ratios of fluid mobile to fluid immobile elements such as Ba/La (65-122), Ba/Th (484-1304) and U/La (0.08-0.17). Additionally, they have $^{143}Nd/^{144}Nd$ (0.51300-0.51307) similar to normal mid-ocean-ridge basalts (N-MORB) from the East Pacific Rise (EPR), but $^{87}Sr/^{86}Sr$ (0.7035-0.7042) ratios are much higher than those found in fresh EPR glasses. Pb isotopic compositions of the samples (e.g. $^{206}Pb/^{204}Pb$ = 18.5-19.0, $^{207}Pb/^{204}Pb$ = 15.52-15.58) form an array between EPR basalts and subducted sediments. The volatile, trace element and isotope data are consistent with mixing of fluids highly enriched in fluid-mobile elements from subducted sediments with a N-MORB-type mantle wedge to produce the Nicaraguan volcanic rocks. In contrast, olivine-hosted melt inclusions (Fo >82) in Costa Rican volcanic rocks show a similar range in H_2O (up to 5.1%) to Nicaraguan inclusions but overall have lower S (0-1340 ppm) and Cl (10-790 ppm) contents. Costa Rican lavas also have lower Ba/La (7-35), Ba/Th (55-338), U/La (0.02-0.12), $^{87}Sr/^{86}Sr$ (0.7035-0.7038) and $^{143}Nd/^{144}Nd$ (0.51292-0.51301) than Nicaraguan lavas, but $^{87}Sr/^{86}Sr$ and Pb isotope ratios (e.g. $^{206}Pb/^{204}Pb$ = 19.02-19.32) are more radiogenic than in Nicaragua and than usually found in fresh EPR MORB. Our data are consistent with the presence of Galapagos Hotspot-type components in the source of the central Costa Rican volcanic rocks, derived from the subducting Galapagos Hotspot Track and from Galapagos-type material entering the mantle wedge through a slab tear or window (Abratis and Worner, 2000; Geology). The estimated volume of volcanic rocks erupted in the last 100,000 years (Carr et al., 1990, Contrib. Min. Pet.; in press, AGU Spec. Pub.) are substantially higher in central Costa Rica than in Nicaragua, suggesting greater productivity of melting beneath Costa Rica. Since the flux of hydrous fluids appears to be similar beneath both arc segments, higher melt productivity beneath Costa Rica could reflect the presence of larger volumes of more fertile, hotter Galapagos-type mantle upwelling through a slab tear or window into the Costa Rican mantle wedge.

V41A MCC: 3006 Thursday 0800h

Birth, Growth, and Death of Magmatic Arcs: Comparisons Among Arcs in Different Settings III *(joint with T)*

Presiding: **T Rushmer,** University of Vermont; **N Petford,** Kingston University

V41A-01 0800h INVITED

Expressions and controls on intra-crustal recycling

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Heat and mass transfer associated with arc magmatism can play a significant role in crustal differentiation. However, the timescales and controls are diverse and poorly understood. To assess the expression of crustal recycling, we will review and compare three examples: the Sierra Nevada, Cascade, and Costa Rica arcs. Coupled basaltic inputs and crustal melting or reaction provides the template for crustal recycling. This process can be dominated by heat and/or fluid transport, and the relative contributions can be difficult to decipher from anhydrous, residual xenoliths and arc magmas. If the crust is young, thin, and mafic (south Cascade arc), low-K compositions dominate. The compositional diversity in the mafic rocks is nearly as great as in the silicic rocks. Wet melting by mantle input is possible, but radiogenic Os signatures limit the addition of primitive basalts and high Mg andesites as mass sources for erupted magmas. If the crust is old, thick, and silicic (Sierra Nevada), crustal recycling is expressed as a sequence of amphibolite-tonalite-granodiorite with amphibolite and granulite facies roots. High-K compositions result from a multi-stage process of "igneous distillation" but the relative roles of true melting and reaction-assimilation has not been resolved. High-K concentration can also be generated in continental arcs where thin, mafic, refractory oceanic crust constitutes most of the crustal column (Costa Rica). We suggest that the presence of high-K silicic magmas in this setting can be reconciled with repeated melting of a young, mafic lower crust, effectively by-passing the existing crustal framework.

V41A-02 0815h

Possible Melts of Delaminating Lower arc Crust Beneath Arcs

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Theoretical models predict gravitational instability of dense igneous cumulates and orthogneisses overlying less dense upper mantle peridotites (e.g., Herzberg et al CMP 83; Kay & Kay Geol Rundsch 91; Jull & Kelemen JGR 01). This is especially likely when cumulates include pyroxenites, and when temperatures fall below $\sim 900^{\circ}$C at pressures greater than $\sim$ 0.7 GPa, leading to transformation of high-Al arc gabbronorite to garnet granulite. This can induce viscous foundering or delamination of the base of the crust. Primitive cumulates and garnet granulites are present in small amounts near the base of the Jurassic Talkeetna arc section in south central Alaska. Recent work suggests that these are remnants of a much larger proportion of primitive cumulates, most of which is missing from the otherwise complete arc section, perhaps due to delamination (Greene et al J Pet submitted; Kelemen et al Treatise on Geochemistry, 03). If delamination of dense lower crustal rocks occurs in arcs, one might expect this component to participate in arc magmatism (Gromet & Silver J Pet 87; Kay & Kay, Tectonophys 93; Kay et al JGR 94). In the western Aleutian island arc, primitive andesites that are light REE enriched and heavy REE depleted, indicative of abundant garnet in their source, may form by partial melting of subducted eclogite, followed by reaction with the mantle during ascent into the arc crust (e.g., Kay, JVGR 78; Yogodzinski, JGR 95; Kelemen et al., AGU Monograph 03). However, Aleutian samples with this garnet signature have depleted isotopic compositions, with both $^{206}Pb/^{204}Pb$ and $^{87}Sr/^{86}Sr$ lower than in Pacific MORB sampled to date. Talkeetna pyroxenites and garnet gabbros generally have U/Pb and Th/Pb less than, and Sm/Nd

and Lu/Hf greater than the MORB source, and with time, Talkeetna lower crust should evolve to isotope ratios more depleted than the MORB source. Anatexis of garnet-bearing lower crustal rocks will produce isotopically depleted, light REE enriched, heavy REE depleted partial melts. Interaction of these granitic melts with surrounding mantle peridotite will raise their Mg# and Ni, and lower SiO_2 to produce andesitic or basaltic hybrid magmas. Moho temperatures in the western Aleutian arc may be relatively low, below 900°C, due to slow convergence and low magma flux, enhancing formation of garnet granulite and subsequent delamination. Lower arc crust formed during early Aleutian magmatism, with the isotopic composition of MORB at 40 Ma and trace element patterns of Talkeetna pyroxenites and garnet granulites, will evolve to yield isotope ratios like those of Miocene and present day Aleutian andesites. Thus, melting of delaminated garnet granulites within the mantle wedge may be a viable alternative to partial melting of subducted eclogite, producing the light REE enriched, heavy REE depleted component in western Aleutian primitive andesites. Tectonic erosion of old arc basement from forearcs, and incorporation of these rocks into the mantle wedge, might have similar consequences.

V41A-03 0830h

4D constraints on melt source-rock input and granite production in continent-continent collision; a case study from a 50 km wide swath through the Himalayan magmatic arc

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Detailed mapping, mountaineering and high resolution remote-sensing data from the Bhutan High Himalaya illustrate rates & / volumes of magmatic arc growth in continent-contintent collsion. Lunana & Gonto La, a 20 km x 30 km area with >3 km relief, provide 3D data for widespread, km-long, Dm-thick, sill- & laccolith-form leucogranites. These peak-forming (>8000 m) Miocene plutons are typical for the ca.2500 km magmatic arc of the India-Asia continental collision. Extrapolation to geo-traverses through peaks to the east (Khula Kangri, Monlakarchung) onto a 30sec DEM provide tight datapoint 3D subsurface control for >4500 km^3, thereby constraining total pluton shapes and volumes. Geochemistry studies indicate exclusively decomposition melting (Harris, et al. 2002) and permit us to calculate required melt-source rock volumes for various conditions. Project INDEPTH seismic reflection profiling (conducted imm. to the N. - Nelson et al. 1996) has been used with further mapping to obtain a 50 km wide, 150 km long swath through the entire orogen. These reveal the sub-surface form of the shallow, gently N-ward dipping, crystalline, mid-crustal layer that is exposed at the High-Himalaya, the upper part of which the plutons intrude. The 4D part of our 3D swath through the magmatic arc is geochronology for the plutons and, to the north, of local granitoid protrusions from beneath the cover rocks of the melted mid-crustal layer that constrain a N-ward younging of plutonism (Copeland 1990; Edwards & Harrison 1997; Edwards et al. 1998; Li et al. 1998). Using these time constraints together with a kinematic model incorporating dilatant flow where both lines of no-rotation are stretching and non-parallel to shearing boundaries, we link deformation with melt source-rock magmatic product volume changes. We derive a timetable for melt addition and thereby rates of magma extraction and ascent.

V41A-04 0845h INVITED

Rifting, Insertial Magmatism And Continental Arc Construction, Peru

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The Mesozoic-Cenozoic tectonic evolution of the Peruvian continental margin of South America is dominated by periods of intracontinental rifting and basin formation. The Andean cycle in this region starts in the Cretaceous with intrusion of the tonalite-dominated Coastal Batholith (CB) into an Albian marine basin forming part of a major extensional system extending from Columbia to the Antarctic. Basaltic material at the bottom of the basin was remelted to produce mainly tonalitic magmas of the CB, which were intruded vertically up axial fractures to form thin, trench-parallel, horizontal intrusions near the surface. Gravity modelling of the CB and its envelope shows the intrusion is tabular, with an aspect ratio close to 20. Individual plutons have aspect ratios close to 5. A thick (10-km) root zone to the west is interpreted as a multiple dyke feeder system. It is likely that much of the CB was intruded under a shallow sea that covered the basinal rocks prior to inversion. From Eocene times onwards, volcanism and plutonism migrated inboard, culminating in the intrusion of the Cordillera Blanca Batholith (CBB) and Yungay ignimbrites at c. 6 Ma. Situated above the now thickened crustal root of the Andes (c. 60 km), the CBB was intruded into Jurassic basinal shales which form part of the much larger West Pervian Trough, and its emplacement overlaps with intense uplift and exhumation along the Andean margin at c. 15-10 Ma. The western margin of the basin and CBB terminate at the Cordillera Blanca fault complex, a deeply disecting, trench-parallel crustal lineament. In contrast to traditional models of cordilleran magmatism, which often predict 'S'-type magmas inboard of the main arc, the CBB rocks are high Na, high Sr/Y types similar to Archean trondhjemites that contrast markedly with the calc-alkaline magmas of the CB. Similar calc-alkaline to adakite-like compositional trends are seen in spatially related volcanic rocks in land from the trench. In the Peru arc, the generation of large volumes of granitic (s.l.) melts is related to periods of crustal extension, with the pre-existing (Gondwana) structural template of the continental margin controlling both location and style of intrusion. The source material for the majority of plutonic rocks was newly generated basaltic lower crust. Volume constraints imply that the crustal column beneath the western Peruvian arc evolved significantly from c. 20 to 5 Ma, with vertical thickening driven by an elevated flux of mantle-derived magma into the lower crust, followed by rapid intracrustal remelting and chemical differentiation. It is likely that flare-up of insertial magmatic activity combined with rifting has led to periodic thermal weakening of the entire arc, resulting in fluctuating bulk rheology of arc lithosphere over time.

V41A-05 0900h

Crustal Architecture and Structural Patterns of the Cretaceous to Paleogene Cascades Arc

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The crystalline core of the North Cascades (Cascades core) preserves a crustal section of ca. 10- to 40 km paleodepths that facilitates evaluation of the crustal architecture and partitioning of strain during major shortening of this 96- to 45 Ma continental magmatic arc. The dominantly tonalitic plutons in the arc are steep-sided, vertically extensive bodies that commonly are sheeted. They intrude oceanic and arc terranes juxtaposed along initially gently dipping thrusts before 92 Ma. Shortening, crustal thickening, and amphibolite-facies metamorphism of the Cascades core were synchronous with large (> 100 km) thrust displacements at shallow levels in the ca. 100-80 Ma NW Cascades thrust system. Deformation in the core was dominated by early tight to isoclinal, gently inclined to recumbent folds that were followed by open to tight, more upright folds. SW-vergent, moderate to steeply dipping reverse shear zones, which postdate terrane juxtaposition, were localized next to plutons. They have < 10 km displacement and were responsible for less shortening than the folding. Metamorphic and geochronologic data indicate rapid burial of plutons and host rocks during the mid-Cretaceous deformation. Shortening in sub-greenschist-facies, ophiolitic rocks above the Cascades core was manifested by upright folds and steep reverse shear zones that reactivated Jurasssic faults inferred to have formed in an oceanic fracture zone. Folding and reverse shear persisted in the Cascades core until at least 65 Ma, well after major thrusting ceased in the NW Cascades system. The younger shortening structures are confined to deeper, more internal parts of the arc, and were probably localized in part by magmatism and thermal weakening. This shortening was also broadly coincident with cryptic thrust burial of sedimentary protoliths of the Swakane Gneiss from the surface to 40 km between 73 to 68 Ma. This underthrusting may have removed the roots of the arc plutons. Similar deformation patterns throughout the crustal section imply structural coupling of large parts of the arc. This coupling may reflect the consistently tonalitic composition (rather than more mafic composition with depth) of plutonic rocks and low paleogeothermal gradients of the section. Structural partitioning was more strongly controlled by relatively localized rheological contrasts, particularly the presence of rigid plutons and other mechanical anisotropy.

V41A-06 0915h

Tectonic evolution of the Notre Dame magmatic arc, Newfoundland Appalachians

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Notre Dame continental arc magmatism in Newfoundland had an overall lifespan of c. 60 Ma (489-429 Ma). Extensive age dating suggests that arc construction took place in 3 distinct stages, separated by gaps of magmatic quiescence (arc shut-off). The first phase of quiescence (c. 480-468 Ma) corresponds to the start of Taconic collision between the initially west-facing Notre Dame arc and Laurentia. The second phase of magmatic quiescence (455-445 Ma) corresponds to collision between the now east-facing Notre Dame arc and the west-facing, peri-Gondwanan Victoria arc built on a piece of Ganderian crust. Resurgence of arc magmatism followed stepping- back of the west-dipping subduction zone into the oceanic marginal basin that separated the Victoria arc from the Gander margin. A gradual transition (431-429 Ma) from arc-like to mainly juvenile, bimodal within plate-like magmatism coincides with suturing of the Notre Dame arc with the Gander margin along the Dog Bay line and probably reflects break off of the west-dipping Ganderian slab. Preservation of an unconformable and unmetamorphosed Silurian cover, consisting of red beds and bimodal volcanic rocks, over large tracts of the Notre Dame arc indicates that the arc was extinct and stabilized by the Late Silurian (c. 425 Ma) and did not experience any significant overprint during the Early Devonian Acadian orogeny, the effects of which were mainly localized further to the east due to accretion of Avalonia to Laurentia. The second, Mid-Ordovician phase of arc magmatism (c. 469-456 Ma) appears most voluminous and was mainly characterized by K-poor, calc-alkaline quartz diorite to tonalite and, to a lesser extent granodiorite, plutons. These calc-alkaline plutons intruded during deformation and significant thickening of the Notre Dame arc, presumably as a result of ongoing shortening following initial collision with Laurentia and an arc-polarity reversal. Such a tectonic scenario is consistent with the high metamorphic grade of the supracrustal rocks they intruded and high La/Yb content of most tonalites, which suggests melting of garnet-amphibolite near the base of an over thickened arc. The first evidence of emergence of the Notre Dame arc following its thickening is provided by unconformably overlying, late Caradoc (c. 453 Ma) subaerial ignimbrite and conglomerate. Parts of the Notre Dame arc show very rapid exhumation of its middle to lower crust at c. 430 Ma, following shortening during the Early Silurian. Exhumation was presumably triggered by slab breakoff during final suturing between Ganderia and Laurentia.

V41A-07 0930h

Crustal Structure and Rock Uplift due to Back-Arc Extension.

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We use crustal structure and exhumation data to estimate the density and partial melt variation in the mantle wedge of a back-arc extension system. A program of explosion seismology (NIGHT) in the central North Island (CNI) of New Zealand has unearthed an intriguing, isostatic contradiction: an association of profoundly thin continental crust with recent rock uplift. We explore properties of the upper mantle that might lead to sufficient buoyancy to compensate the

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thin crust and raise the solid surface of the CNI into a lithospheric dome. Andesite and rhyolite volcanism have been present in the CNI for the past 4-5 my. Mudstone porosity analyses to the west and south of the volcanic region shows that over 2 km of exhumation has occurred in CNI since 4 Ma. This combined with a coeval surface uplift of ~ 500 m, indicates a maximum 2.5 km of rock uplift. Marine terraces 100-150 km from the centre of maximum exhumation show uplift rates of ~ 0.2-0.3 mm/y consistent with about 1 km of exhumation if averaged over 4 my, which compares well with the mudstone porosity results. The magnitude and wavelength (~ 400 km) of the uplift is similar to that observed in continental areas associated with mantle upwelling (e.g. Yellowstone). Explosion seismic studies show an arched Moho, crust that has been thinned to nearly half its original thickness and Pn wave-speeds 8% lower than normal. Seismic attenuation (Q) studies show strong attenuation throughout the mantle wedge below CNI. Isostatic modelling is used to explore processes consistent with these observations. The observed rock uplift pattern may be explained by the replacement of about 70 km of mantle lid with asthenosphere of density contrast ~ 100 kg/m^3 with respect to normal mantle. Such a density contrast cannot be explained by temperature change alone, and a partial melt of up to 5% is implied. Strong seismic reflections from within a confined zone of the mantle wedge were recorded. These reflections from ~ 35 km deep show strong amplitudes in an incident angle range consistent with the AVO response of a body with a high degree of fluid or melt.

V41A-08 0945h

Transient Dilatancy in the Transport of Magma and Flareup Magmatic Events

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Migmatite belts around the world show features that have led workers to conclude that melts move into strain heterogeneities such as boudin necks and shear zones. The inference generally made is that these are transient sites of relatively low pressure. In the Main Martir Thrust zone of the Peninsular Ranges batholith, synkinematic migmatites formed in a kinematically well-constrained setting. Melt layers on the thrust zone occupy shear bands and are connected across short jogs at a high angle to the thrust-zone boundaries. This geometry is analogous to dilatant jogs that form between interacting brittle cracks. The formation of these features at elevated T suggests that elevated strain rates, elevated magma pressures, or both played an important role in embrittlement. Magmatic arcs are commonly long-lived, but their construction is apparently dominated by a limited number of transient magmatic events. In the Peninsular Ranges batholith, approximately 50% of the exposed arc was emplaced between 99 and 92 Ma, leading to production rates on the order of 75-100 km*3/km/m.y. Several different explanations have been proposed for such transient flareup events, and here we explore, in 3-D, the implications of crustal-scale dilatancy to magma formation and transport processes during lithospheric subduction, using the North Island of New Zealand as a modern analog.

V41B MCC: 3008 Thursday 0800h

Frontiers in High-Pressure Research: New Opportunities I *(joint with GP, MR, DI)*

Presiding: **A B Belonoshko,** Royal Institute of Technology**; Y Zhao,** Las Alamos National Laboratory

V41B-01 0800h INVITED

Scientific Advancements and Technological Developments of High P-T Neutron Diffraction at LANSCE, Los Alamos

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In-situ high P-T neutron diffraction experiments provide unique opportunities to study the crystal structure, hydrogen bonding, magnetism, and thermal parameters of light elements (eg. H, Li, B) and heavy elements (eg. Ta, U, Pu,), that are virtually impossible to determine with x-ray diffraction techniques. For example, thermoelasticity and Debye-Waller factor as function of pressure and temperature can be derived using in-situ high P-T neutron diffraction techniques. These applications can also be extended to a much broader spectrum of scientific problems. For instance, puzzles in Earth science such as the carbon cycle and the role of hydrous minerals for water exchange between lithosphere and biosphere can be directly addressed. Moreover, by introducing in-situ shear, texture of metals and minerals accompanied with phase transitions at high P-T conditions can also be studied by high P-T neutron diffraction. We have successfully conducted high P-T neutron diffraction experiments at LANSCE and achieved simultaneous high pressures and temperatures of 10 GPa and 1500 K. With an average 3-6 hours of data collection, the diffraction data are of sufficiently high quality for the determination of structural parameters and thermal vibrations. We have studied hydrous mineral (MgOD), perovskite (K.15,Na.85)MgF3, clathrate hydrates (CH4-, CO2-, and H2-), metals (Mo, Al, Zr), and amorphous materials (carbon black, BMG). The aim of our research is to accurately map bond lengths, bond angles, neighboring atomic environments, and phase stability in P-T-X space. Studies based on high-pressure neutron diffraction are important for multidisciplinary science and we welcome researchers from all fields to use this advanced technique. We have developed a 500-ton toroidal press, TAP-98, to conduct simultaneous high P-T neutron diffraction experiments inside of HIPPO (High-Pressure and Preferred-Orientation diffractometer). We have also developed a large gem-crystal anvil cell, ZAP-01, to conduct neutron diffraction experiments at high-P and low-T. The ZAP cell can be used for integrated experimental techniques of neutron diffraction, laser spectroscopy, and ultrasonic interferometry. We are conducting further developments of high P-T technology with a new 2000-ton press, TAPLUS-2000, and a ZIA anvil package to achieve of pressure of 30 GPa and temperatures of 3000 K. The new design of a dedicated high pressure neutron beamline, LAPTRON, is also underway for simultaneous high P-T neutron diffraction, radiography, and tomography studies. We seek strong community support for this new development.

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X-Ray Microdiffraction at Megabar Pressures

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High-pressure x-ray diffraction (XRD) provides unique, important sources of structural information of minerals in the Earth's deep interior, but encounters major limitations. The restriction to forward diffraction geometry (2θ less than 90°) severely limits the accuracy. With the 50-5 μm size x-ray beam typically used to probe samples at 30-200 GPa, the number of crystals covered by the x-ray beam is often too few for good polycrystalline XRD, but too numerous for single-crystal XRD. Single-crystal XRD method with monochromatic x-ray source and 2-d detector works satisfactorily for crystal size larger than 20 μm, but when the crystal is significantly less than 5 μm, the sample signals are often overwhelmed by the background. Energy dispersive XRD with polychromatic x-radiation has been used successfully to determine unit-cell parameters of smaller single crystals, but the intensity information is unusable for structural refinement because this method requires rotation of the small crystal relative to the small x-ray beam. Recent integration of panoramic diamond anvil cell[1] (PDAC) with synchrotron x-ray microdiffraction[2] (XRMD) method has finally overcome these limitations and can potentially revolutionize the high-pressure XRD field. This XRMD method focuses polychromatic x-radiation to submicrometer size to resolve very small single crystals, and collects Laue spots with a 2-d CCD detector. The PDAC allows complete forward, 90°, and back scatterings, while the background signal is minimized by directing the incident x-ray beam through single-crystal diamonds (i.e., avoiding the beryllium seats and gasket). The incident beam can be changed to monochromatic, tuned through the full energy (wavelength) range, and focused to the identical submicrometer spot for d-spacing determination of each Laue spot. All polychromatic Laue spots are collected simultaneously from the same x-ray sampled volume, thus reliable for structure determination. The development provide long-sought solutions to important technical and scientific issues, including the fundamental changes of silicates, oxides, ices, and condensed gases that are the main components of deep planetary interiors. [1] H. K. Mao, J. Xu, V. V. Struzhkin, et al., Science 292, 914 (2001). [2] N. Tamura, R. S. Celestre, A. A. MacDowell, et al., Rev. Sci. Instrum. 73, 1369 (2002).

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High-pressure and High-temperature Studies With Nuclear Resonant Scattering

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In this contribution, we report the extention of nuclear resonant scattering techniques into the high-pressure and high-temperature sector relevant to the geophysical problem area. Nuclear resonant scattering techniques that utilize synchrotron radiation have provided new opportunities for the study of vibrational properties, magnetic properties, and iron valancies of condensed matter under extreme conditions. Here we will address nuclear resonant inelastic x-ray scattering (NRIXS), a method that uses probe nuclei with suitable resonances to measure the vibrational density of states, and synchrotron Mössbauer spectroscopy (SMS) for determination of valancies. Both methods are very sensitive to small amounts of material and take advantage of the high brilliance of synchrotron radiation, which makes micrometer-sized x-ray beams with high intensity possible. These properties allowed NRIXS and SMS investigations on materials under pressures in the Mbar regime using diamond anvil cells [1,2]. In general, NRIXS provides the phonon density of states [3] and sound velocities [4], whereas SMS gives access to the abundance of ferric iron in lower mantle polymorphs [2]. The introduction of Laser heating in combination with NRIXS and SMS at sector 3-ID of the Advanced Photon Source permits us now to conduct these studies under high pressure *and* high temperature. First results on iron metal and iron-containing perovskite $Fe_{0.1}Mg_{0.9}SiO_3$ up to 50 GPa and 1500 K will be presented to exemplify the usefulness of these novel techniques. This work is supported by the U.S. DOE-BES, Office of Science, under Contract No. W-31-109-Eng-38. [1] H.K.Mao, J.Xu, V.V.Struzhkin, J.Shu, R.J.Hemley, W.Sturhahn, M.Y.Hu, E.E.Alp, L.Vocadlo, D.Alfe, G.D.Price, M.J.Gillan, M.Schwoerer-Böhning, D.Häusermann, P.Eng, G.Shen, H.Giefers, R.Lübbers, G.Wortmann, Science **292**, 914 (2001) [2] J.M.Jackson, W.Sturhahn, G.Shen, J.D.Bass, (unpublished) [3] W.Sturhahn, T.S.Toellner, E.E.Alp, X.Zhang, M.Ando, Y.Yoda, S.Kikuta, M.Seto, C.W.Kimball, and B.Dabrowski, Phys.Rev.Lett. **79**, 3832 (1995) [4] M.Y.Hu, W.Sturhahn, T.S.Toellner, P.Mannheim, E.E.Alp, Phys.Rev. B **67**, 094304 (2003)

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Solid-Solid Transitions at High-PT: Implications for the Earth's Core

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Solid-solid (s-s) transtions can be separated in two groups: one pressure (P) induced and second temperature (T) induced. We will call P-induced s-s transitions those which occur on increasing the pressure (normally at low T) and T-induced s-s transitions those which occur on increasing T at a given P. While P-induced s-s transitions comparably easy to detect experimentally, T-induced s-s transitions might occur at such a high T