significant Fe^{3+} was detected. The δ/Fe and ΔE_q are in good agreement with literature data. The thickness effect for our measurements is negligible as the effective thickness at most was ~0.3 mg Fe/cm^2. The distribution coefficient K_D is calculated from Fe(M1)/Fe(M2) ratio determined by Mössbauer spectroscopy taking into account of minor elements. The uncertainty (2σ) on K_D values ranges from 0.007 to 0.025. The calculated K_D as function of temperature can be expressed as: $\ln K_D = 0.381\ (\pm 0.067) - 2236\ (\pm 70)/T(\mathrm{K})$. Compared to previous studies, our results show much less nonideality for Fe-Mg mixing between M1 and M2 sites in Mg-rich orthopyroxenes.

T32G-05 1430h

Iron and Manganese Substitutions in Olivine

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There are many questions remaining regarding olivine in the mantle. The distribution of iron and manganese between the two magnesium sites has been the subject of much experimental study, due to its potential applications as a geospeedometer. However, neutron-diffraction studies have yielded quite different results, indicating either an ordering or a disordering of the elements between the two sites. A computer simulation study of Fe^{2+} and Mn^{2+} substitutions in olivine has been carried at 0-15GPa and temperatures to 1500K. The aim has been to calculate the substitution energies associated with the incorporation of Fe^{2+} or Mn^{2+} into the two magnesium sites to identify which substitutions are most energetically favourable over the range of mantle conditions. Results indicate that, energetically, it is most favourable for both Fe^{2+} and Mn^{2+} to enter the Mg2 site when the species are introduced into forsterite, whereas for olivine of composition $(Fe,Mn)_2SiO_4$ it is most favourable for Fe^{2+} to enter the Mg1 site and Mn^{2+} to enter the Mg2 site. This is valid for all pressures and temperatures considered, indicating that ordering remains favourable over mantle conditions.

In addition, the energies associated with Fe^{3+} entering the Mg or Si sites and vacancies on the Mg, Si or O sites in forsterite have been determined. Results from this have been used, in comparison with previously determined energies for ferric iron substitution mechanisms in perovskite, to address the issue of why the incorporation of ferric iron in olivine is unfavourable relative to perovskite. It has been found that the most favourable mechanism for the incorporation of ferric iron into perovskite is Fe^{3+} entering both the Si and Mg sites, directly charge balancing each other and thus avoiding energetically costly vacancies. Although this is also the most favourable mechanism for forsterite, it is less favourable by approximately 3eV. This is due to Fe^{3+} substitutions into the Si site being significantly more energetically costly in olivine compared with perovskite. In fact it is almost the same energetically as putting Fe^{3+} into the M1 site only and charge balancing by cation vacancies, which explains why so little Fe^{3+} enters forsterite.

T32G-06 1445h

Thermoelastic Interpretation of Internal Pressure Imposed on an (Mg,Fe)O Inclusion in Diamond: Support for a Deep Mantle Origin

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The presence of mineral inclusions of (Mg,Fe)O (fPer) within diamonds and particularly their association with $(Mg,Fe)SiO_3$ inclusions, is considered to be evidence for formation within the Earth's lower mantle (e.g. Harte and Harris, 1994). The structural state of fPers can be used as independent evidence for a depth of origin for their occluding diamonds. Cell parameters of a Guinean fPer inclusion (GU4A) were measured by X-Ray diffraction before and after release from its host diamond. Analysis was performed at the University of Edinburgh using a Gandolfi camera with a MoKα X-Ray source of beam size greater than that of the inclusion (180 μm). Average cell parameters were found to have increased significantly subsequent to release (4.2288 to 4.2397 Å; ±0.2%) which, given the thermoelastic properties of GU4A composition fPer (interpolated from published data for MgO and FeO end members), corresponds to a confining pressure within diamond of 1.29 ±0.38 GPa. A 3rd order temperature dependent Birch Murnaghan EOS, and published thermoelastic data for diamond were used to model the build-up of internal pressure on GU4A composition fPers on exhumation along two mantle geotherms. Results show that assuming no internal pressure was released by brittle fracture of the host diamond, the internal pressure surrounding GU4A corresponds to a minimum possible formation depth of 320 ±22 km, i.e. within the transition zone. However, the diamond around GU4A was observed to be fractured (Hutchison, 1997) and, although no accurate value is known for how much pressure was released by such fracture, a conservative estimate based on SEM study of displacement of fPer grain boundaries of a similar stone, increases the minimum depth of formation for this diamond to within the lower mantle.

Internal pressure imposed on this fPer inclusion, therefore, concurs with Mössbauer measurements on São Luiz diamonds (McCammon et al., 1997) which conclude that fPer-bearing diamonds cannot have formed at shallow depth under unusual oxidation conditions.

Harte, B. and Harris, J. W. (1994) *Min. Mag.* **58A**, 384-385

Hutchison, M. T. (1997) PhD. Thesis, Univ. Edinburgh

McCammon et al. (1997) *Science* **278**, 434-436

T32H MC: 122 Wednesday 1515h
Fluid Flow in and Physical Properties of Porous Rocks II *(joint with H, S)*

Presiding: **J T Fredrich**, Sandia National Laboratories; **B Kaelin**, Lawrence Berkeley National Laboratory

T32H-01 1515h

Microscale Flow Modeling in Reconstructed Porous Media

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We describe how recent developments in 3D imaging techniques, numerical methods for simulating flow and transport, and emergent computational architectures are combined to enable numerical studies of fluid flow in complex porous media. High-resolution volumetric image data of porous geomaterials are obtained using laser scanning confocal microscopy. The pore space of a core sample is impregnated with a low viscosity epoxy doped with a fluorochrome that is excited under laser illumination. Volumetric image data, consisting of fluorescence intensity for typically ~50 million voxels in XYZ space, are segmented into void and solid phases from which the 3D structure of the two-phase medium can be reconstructed. The binarized image data may be analyzed to quantify various geometric attributes, and used to automatically generate a mesh for numerical flow simulations. The principal issue regarding the tractable computation of transport phenomena in the reconstructed porous medium lies in the complexity of the geometry and the retention of this structure in numerical analyses. Lattice Boltzmann Methods (LBM) have arisen as the most attractive approach for simulating transport processes in complex geometric domains due to the method's unique ability to simply and efficiently treat the multitude of discrete boundary conditions. LBM are extremely accurate, but computationally very expensive in both space and time. However, because LBM is a numerically explicit scheme, distributed computing methods can be efficiently applied to the problem. 3D single-phase flow simulations using reconstructed porous media have been performed using the ASCI-Red massively parallel supercomputer. More recently, algorithmic developments, and in particular use of a stencil representation for the two-phase medium, have allowed production-scale simulations to be performed on a purpose-built distributed processor system consisting of 24 processors with a high bandwidth communication switch. The simulations can be used to predict macroscopic properties such as permeability, and volume visualization software is used to study the 3D flow geometry in the complex geometric domains characteristic of porous geomaterials.[a]

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T32H-02 1530h

Laboratory Observations of Fluid Flow Stimulation in Porous Rocks During Dynamic Stress Excitation

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In laboratory experiments, our work shows that application of low-frequency stress excitation can stimulate fluid flow in porous rocks. In the experiments, a Berea sandstone core (2.5 cm × 32 cm) was placed under independent radial and axial confinement. The permeability of the core to brine solution (3 wt% sodium chloride solution) was 800 millidarcy; the connected pore volume was 38 cm^3. In the experimental setup, brine and decane are pumped through the core using two separate pumps producing virtually pulse-free flow. Low-frequency stress oscillations are applied to the core using a magnetostrictive actuator.