

Environmental, Earth, and Extreme Conditions Sciences

SRI 2015 Satellite Workshop

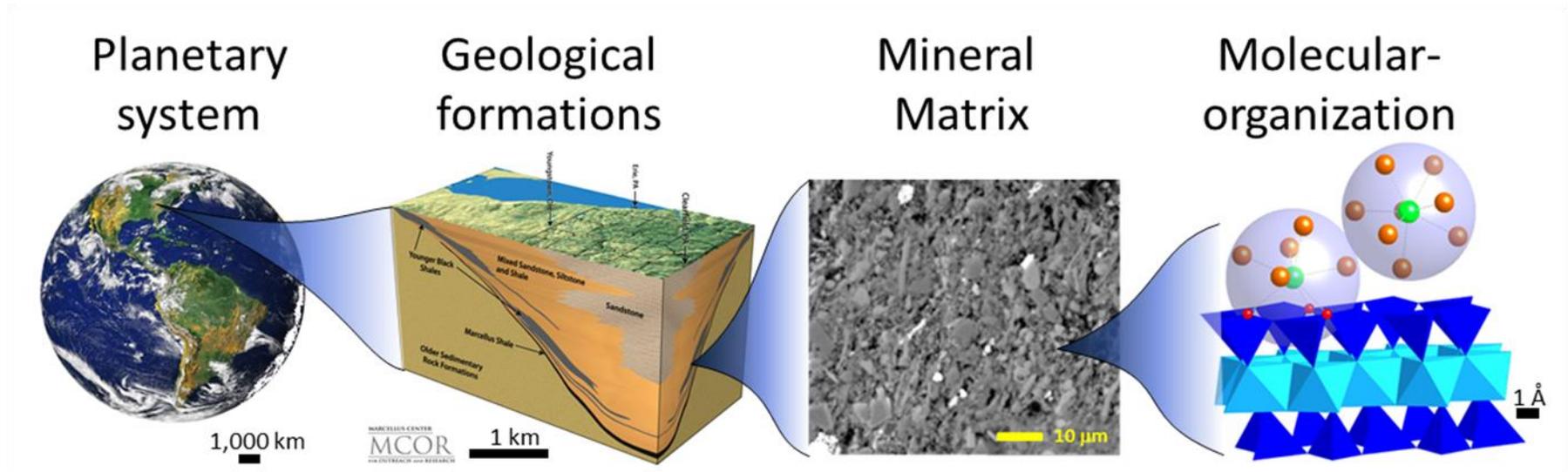
Contributions from members of the E³ communities

E³ APS-MBA Workshop, June 2015

Opportunity for members of the E³ community to identify compelling science that will take advantage of APS-U properties. Workshop report to be part of APS-U early experiments document.



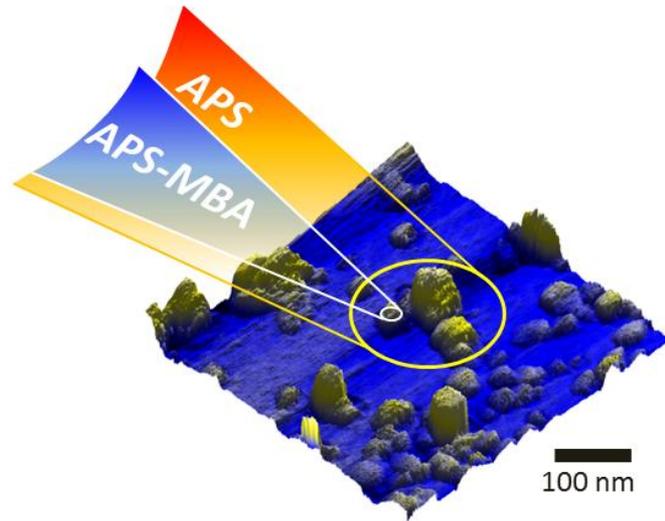
Extremes – scale and heterogeneity



Geosystems inherently display extreme heterogeneity ranging from molecular to planetary length-scales (and beyond . . .)

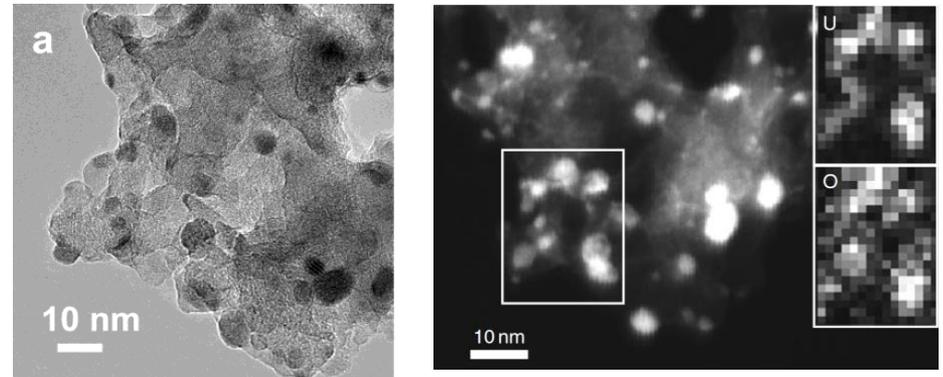
Rich opportunity at the interfaces

Environmental – submicron contaminants



Ex-situ atomic force microscopy image of PuO_2 -nanoparticles formed spontaneously at the muscovite-water interface.
(From Schmidt et al., *Environ. Sci. & Tech.*, 2013)

Current interfacial X-ray microscopy limited to ~100 nm (orange circle). The APS-U will achieve a substantially improved spatial resolution through coherent diffraction (<20 nm, in blue).

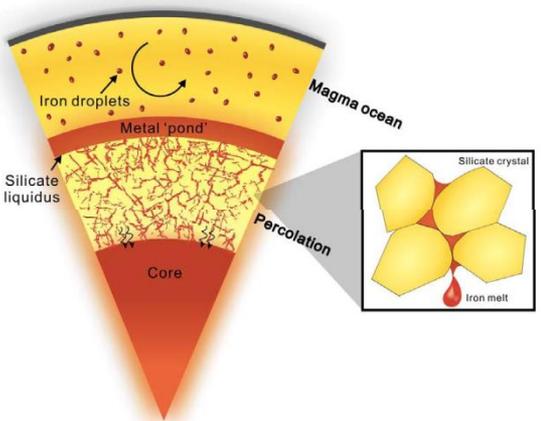


Uraninite nanoparticles in atmospheric particulates (a) BF-TEM shows small heavy particles within the carbonaceous matter of soot less than 10 nm in size. Insets are elemental maps of U and O by STEM-EDX.

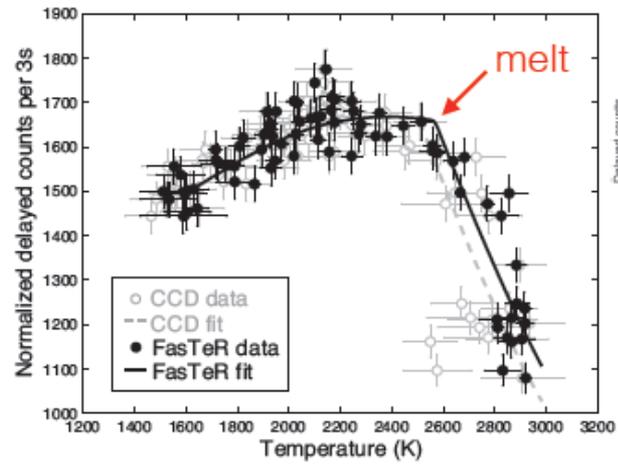
Utsunomiya et al. (2002, 2004)

MBA upgrade will allow XAFS of nm sized metal-rich domains in atmospheric dust.

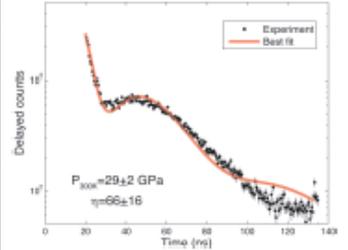
Earth – iron remains a grand challenge



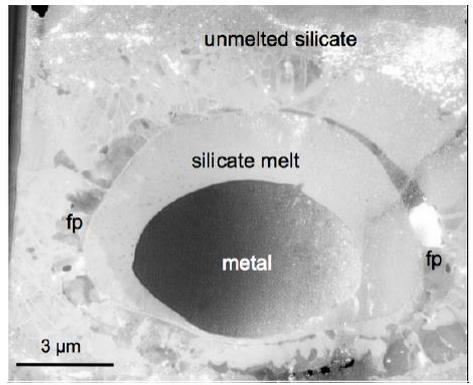
C. Shi et al, Nature Geoscience (2013)



SMS spectrum



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57 GPa, 4400 K (Fischer et al., submitted)

MBA upgrade will offer high resolution x-ray microprobe to characterize samples representing lower mantle and core assemblages

Ideally, would use 3D x-ray fluorescence mapping to fully characterize sample.

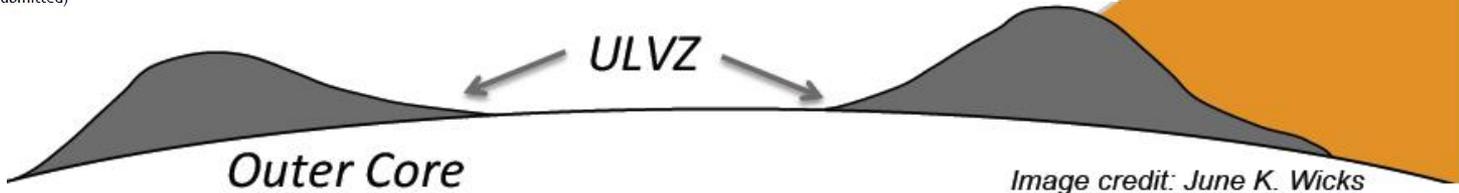


Image credit: June K. Wicks

Extreme conditions – beyond the Geotherm

Hydrogen and the other light elements remain grand challenges

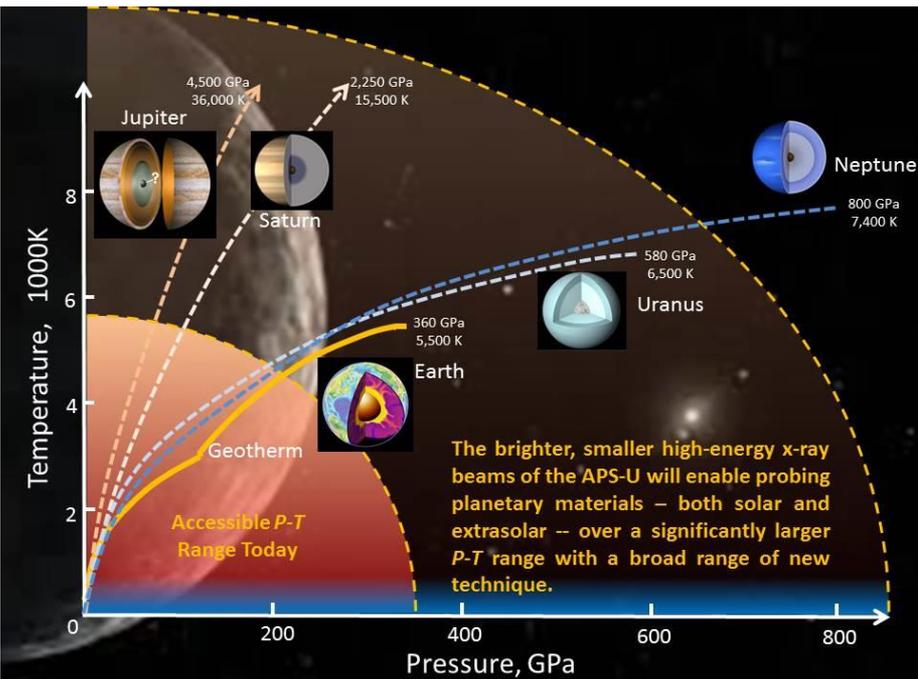
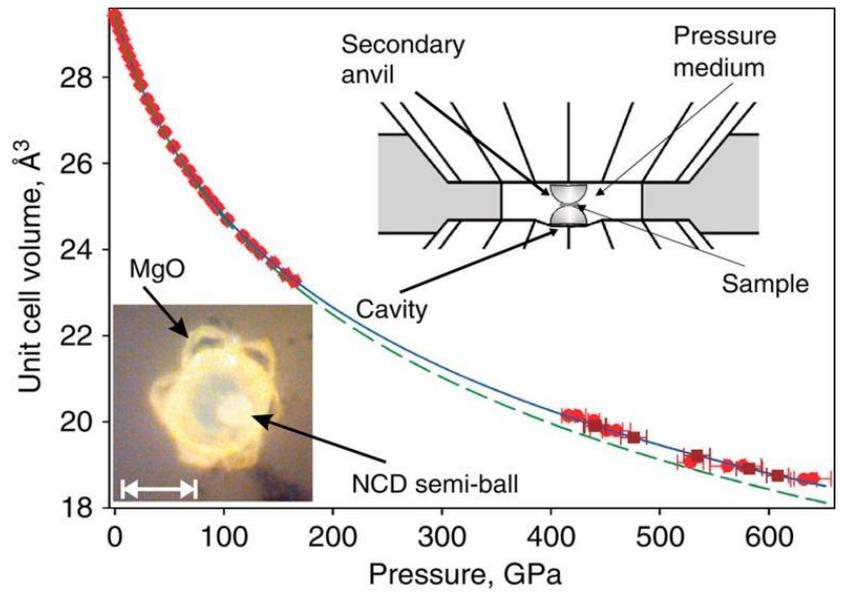


Figure courtesy of Guoyin Shen

With 100x brightness we will be able to observed XRD from the lightest element hydrogen to make structural determinations at ultrahigh pressure

MBA upgrade will allow for sub-micron beam (without loss of photon flux) to mitigate extreme pressure gradients



Dubrovinsky et al. Nature Comm. (2012)

Needs - checklist

- ❑ Storage ring – diffraction limited performance
- ❑ X-ray source – highest-flux undulators (preferably with canted operation)
- ❑ Front end – ultra-stable (mechanical, thermal) monochromator options
- ❑ Focusing optics – easy-to-use, high efficiency, wavelength independent
- ❑ Sample environment – stable, submicron positioning in modified environments
- ❑ Detectors – high-efficiency, high spatial and energy resolution
- ❑ Software – on-the-fly, automated processing of large volumes of imaging data

Obsolete Software Decision Matrix

	Replacement cost			Backward compatibility		Productivity drop			
	Money is no Object	Limited Funds	Not an Option	Don't Care	Convert Existing Data	Must Have	Acceptable	Retraining Permitted	Unacceptable
Upgrading the computer's operating system, or some part of it	Purchase new software or upgrade existing software.	Try to find a replacement tool within budget. If needed, find an older machine.	Find an older machine with compatible operating system.	Don't base any decision on existing data.	If replacing software, make sure it has conversion tools.	Find an older machine with compatible operating system.	Don't base any decision on loss in productivity.	Try to find a replacement within budget that builds on users' skill set.	Find an older machine with compatible operating system.
Upgrading software that depends on the now-broken tool	Purchase new software or upgrade existing software.	Try to find a replacement tool within budget. If needed, find an older machine.	Rollback that upgrade!	Don't base any decision on existing data.	If replacing software, make sure it has conversion tools.	Rollback that upgrade!	Don't base any decision on loss in productivity.	Try to find a replacement within budget that builds on users' skill set.	Rollback that upgrade!
Limits exceeded, e.g., number of records the tool can save	Purchase new software or upgrade existing software.	Before searching for a replacement tool, consider archiving inactive records.	Search web for possible work-arounds, consider archiving inactive records.	Don't base any decision on existing data.	If replacing software, make sure it has conversion tools.	If replacing software, make sure it has conversion tools.	Don't base any decision on loss in productivity.	Try to find a replacement within budget that builds on users' skill set.	If the data can't be archived, decision must be based on other factors.
Our workflow changes	Purchase new software that better suits our needs.	Purchase new software that better suits our needs.	Search web for possible work-arounds, reanalyze workflow.	Don't base any decision on existing data.	If replacing software, make sure it has conversion tools.	If replacing software, make sure it has conversion tools.	Don't base any decision on loss in productivity.	Try to find a replacement within budget. New skills may be required.	Replacement tool must be compatible in functionality to old tool!
We outgrow the tool	Purchase new software that better suits our needs.	Purchase new software that better suits our needs.	Rethink everything	Don't base any decision on existing data.	If replacing software, make sure it has conversion tools.	If replacing software, make sure it has conversion tools.	Don't base any decision on loss in productivity.	Try to find a replacement within budget. New skills may be required.	Rethink everything

Summary

- The Earth, Environmental and Extreme Conditions Science (E³) communities directly benefit from the continued improvements in brilliance afforded by next-generation X-ray storage rings. APS-MBA will further expand the E³ community (atmospheric, oceanographic, and marine science, surface and sub-surface colloidal chemistry).
- Perhaps more than any other scientific discipline, E³ research is highly challenged by the extremely heterogeneous nature of materials studied.
- The unparalleled brightness and coherence afforded by the planned APS MBA upgrade will allow for dynamic, in-situ, and multimodal analysis of heterogeneous E³ materials that is not currently possible.