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Potential of HESEB Soft X-Ray Beamline for Applications in Sustainable Construction Materials

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Introduction

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- . Ordinary Portland Cement (OPC) production alone accounts for 7% of the global carbon emissions [1].
- Reactive Magnesia Cement (RMC), MgO, is a potential low-carbon alternative to OPC.
- . It is currently being produced by one of two ways [2,3]:
 - 1.Calcination of MgCO₃
 - 2. From seawater or desalination reject brine
- RMC absorbs CO₂ through its hydration and carbonation processes [2,3].
- . The resulting hydrated magnesium carbonates form cohesive binding agents akin to that of cement paste [2,3].
- Depending on RMC composition and CO_2 curing conditions, various polymorphs of hydrated magnesium carbonates (HMCs) can precipitate that govern the strength of RMC-based concretes (nesquehonite, dypingite, hydromagnesite, artinite, magnesite) [2,3].
- . The resulting densification and strength vary significantly depending on

Limitations of Current Methodology

Limitations with the laboratory in- situ TEM	How they can be overcome using HESEB Soft X-ray Beamline
Carbon contamination due to the deposition of carbonaceous compounds on sample surfaces under the electron beam irradiation	The low energies of soft x-rays will not cause deposition of carbonaceous layers on samples
Sample damage caused by the high- intensity electron beam	Although there is still a potential for radiation damage to occur with soft x-rays, it is much lower than the damage effect from the high- intensity electron beams of TEM
Limited pressures inside gas cell – maximum of 1 atm	(Depends on available system specifications)
Limited allowance for sample size – maximum gas cell spacer size of 5 µm	Possibility for larger allowance in sample size
Inability to characterize amorphous compounds	Possibility for differentiating amorphous magnesium carbonate

the type and quantity of the precipitated HMC phase [2,3].

Research Objectives

. To guide the nucleation and growth pathways to precipitate highdensity magnesium carbonate phases through the exploration of interfacial energies between reaction products and non-reactive seeds. . The first step is to understand the nucleation and growth mechanisms driving the precipitation of HMCs, which would ultimately pave the path toward the formation of a specific HMC polymorph.

Methodology

- . In-situ Transmission Electron Microscopy (TEM) experiments were conducted on magnesium oxide samples to observe the hydration and carbonation reactions.
- A gas mixture of 20% H_2O and 80% CO_2 was used at 70 Torr pressure and a maximum flow rate of 0.1 sccm.
- The experiments were conduced at 25°C, 50°C and 250°C.

Initial Results

- Carbon contamination was observed at the lower temperatures of 25°C and 50°C which is induced by the electron beam irradiation resulting in the deposition of carbonaceous compounds on the sample surface.
- . Maintaining a higher temperature of 250° C helped avoid the carbon contamination.
- Fractal growth observed at 250°C, which was highly stimulated by the high-intensity electron beam.

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from other crystalline magnesium carbonates (hydrated and anhydrous) based on their different binding energies

Potential Applications

Potential Applications for RMC:

- Possibility of identifying the different magnesium carbonate phases from the detected oxidation states of magnesium ions [4].
- . Potential for near contamination-free sample by cleaning the sample surface and maintaining its cleanness under the ultra-high vacuum conditions [5].
- . Ability to study surface changes on the sample with high resolution using electron and low-energy photons [6].
- . RMC has high water demand and requires chemical admixtures to obtain good workability. Some additives, such as nanoparticles, can also enhance the mechanical and durability properties of RMC. Soft xrays can be used to observe the physical change of RMC under hydration and/or carbonation with/without the presence of polycarboxylate ether (PCE)-based admixtures, Hydroxypropyl methylcellulose (HPMC) polymer, or nanoparticles such as titanium dioxide (TiO₂) and nano-silica (SiO₂).
- . RMC reacts with amorphous silica to produce magnesium silicate hydrates (M-S-H) for which the structure depends on a number of factors such as Mg/Si ratio, reactivity of silica, MgO, alkalinity etc. Soft x -rays can be used to understand the dissolution, nucleation, and growth processes involved in the formation of the M-S-H. Comparisons can also be made with calcium silicate hydrates (C-S-H), which are the common hydration products of Ordinary Portland Cement (OPC).

Other Applications for Sustainable Construction Materials:

. Under a high pH environment, a thin layer of corrosion products of iron

After about 4.5 hours of exposure to gases at 250°C, and no direct exposure to the electron beam

2O(21.14%)/CO2(78.86 ow Rate: 4.577<u>E-08 scc</u>



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beam

exposure

oxides and oxy-hydroxides forms on the steel rebar surface in concrete. Thus, pastes with different pore solution chemistries are expected to create films of different electrochemical, atomic, and protective properties. Soft x-rays can be used to investigate the elemental profile and oxide state of the passive films on the steel rebar surfaces.

. Micro-CT scanning has been used to retrieve 3D models of aggregates that closely resemble lunar regolith. Yet, the quality of the meshes suffers from voxel size. Soft x-rays can be used to retrieve 3D models of lunar regolith simulants and assess the 3D geometry and morphology of aggregates with high-quality meshes.

References

[1] T. Fransen *et al,* "Toward a Tradable Low-Carbon Cement Standard: Policy Design Considerations for the United States," 2021.

[2] Al-Tabbaa, A. (2013). Reactive magnesia cement. In Eco-efficient concrete (pp. 523-543). Woodhead Publishing.

[3] Walling, S. A., & Provis, J. L. (2016). Magnesia-based cements: a journey of 150 years, and cements for the future?. *Chemical reviews*, *116*(7), 4170-4204.

[4] Sedigh Rahimabadi, P., Khodaei, M., & Koswattage, K. R. (2020). Review on applications of synchrotron-based X-ray techniques in materials characterization. X-Ray Spectrometry, 49(3), 348-373. [5] Liu, X., Yang, W., & Liu, Z. (2014). Recent progress on synchrotron-based in-situ soft X-ray spectroscopy for energy materials. Advanced Materials, 26(46), 7710-7729. [6] Yang, F., Feng, X., Liu, Y. S., Glans, P. A., & Guo, J. (2021). In situ/operando soft x-ray spectroscopy

of chemical interfaces in gas and liquid environments. MRS Bulletin, 46(8), 747-754.