

behavior of SiOC will be discussed: (i) the incorporation of carbon into the SiOC glass network leads to an increased creep resistance and viscosity in comparison to vitreous silica. It is shown that the viscosity of a SiOC glass ceramic without segregated carbon phase is higher than the theoretical apparent viscosity of a SiO₂/SiC composite. This is discussed in terms of the interface between SiC particles and the amorphous SiO₂ matrix. (ii) The incorporation of a segregated carbon phase leads to an additional increase in viscosity. Furthermore, the effect of the chemical composition and microstructure (single-phasic and phase-separated) of SiOC glasses and glass ceramics on their elastic properties (Young's modulus, Poisson ratio), hardness as well as their thermal conductivity will be presented and discussed. Their behavior is in accordance to the degree of connectivity of the glass network.

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(PACRIM-S4-014-2017) A low temperature study of magnetic properties of polymer derived SiCN ceramics, doped with Fe ions

S. K. Misra^{*2}; S. I. Andronenko¹; A. Rodionov¹; I. Gilmutdinov¹; R. Yusupov¹

1. Kazan Federal University, Physics, Russian Federation
2. Concordia University, Physics, Canada

SiCN ceramics doped with 3-d transition ions is a new class of materials exhibiting superparamagnetic behavior. They are potentially useful in developing high-temperature magnetic sensor devices. Magnetic properties of polymer derived SiCN ceramics, annealed at 800° C, 1000° C, 1100° C, 1285° C, 1400° C, and activated with Fe (III) acetylacetonate, were investigated at liquid-helium temperatures. The magnetization of SiCN ceramics, activated with Fe ions, annealed at different temperatures, was measured in the range from 4 K to 400 K as a function of temperature ZFC (zero field cooling) and FC (field cooling). It was found that the blocking temperature strongly depends on annealing temperature. The magnetization and X-band EPR were measured as a function of magnetic field at temperatures from 4 K to 120 K. An unusual behavior of the hysteresis curve (butterfly-like) was found in the temperature range just above the blocking temperature. SiCN/Fe ceramics reveal superparamagnetic behavior due to various sources, mainly due to nanoparticles of Fe₅Si₃ and Fe₃Si, as well as due to Fe₇₀Si_xC_{30-x} nanoparticles, dispersed in SiCN nanoceramics. This research was supported by the Natural Sciences and Engineering Research Council of Canada (NSERC) (SKM); SIA is grateful to Ministry of Education of Russian Federation, for partial support in the frame of project, allocated to KFU.

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(PACRIM-S4-015-2017) Physical properties and thermal resistance of Si-O-C(H) ceramics obtained by polysiloxane pyrolysis

M. Narisawa^{*1}; S. Takeuchi¹; K. Sasakawa¹; T. Kawai¹; H. Inoue¹

1. Osaka Prefecture University, Japan

Ceramic yields of linear polysiloxanes are generally low because of cyclic oligomer repulsion process during the heating. In order to increase the ceramic yields, a dense cross-linked structure, which prevents the bond rearrangement process, is necessary. Introduction of vinyl or phenyl groups in original molecular structure is also known to be effective for increasing the apparent ceramic yields. There is, however, the concern that during pyrolysis such side groups are converted to free carbon domains. In an inert atmosphere, once formed SiOxCy materials from polysiloxanes are considered to be decomposed beyond 1,400 °C. If the free carbon content in the Si-O-C material is high, SiC and excess carbon are formed during the carbotherminal reduction. On the other hand, our group in Osaka Prefecture University succeeded in synthesis of "white" SiOxCy materials, which contained almost no free carbon, by using hydrogen for a pyrolysis atmosphere of a kind of polymethylsiloxane. Behaviors of such "white" SiOxCy materials at high temperature beyond 1,400 °C in various atmosphere were

investigated, and obtained results were analyzed in terms of thermodynamic calculation. Recent try of using hydrogen for pyrolysis of the polysiloxanes which contains a high amount of phenyl groups will be also introduced as a recent topic.

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(PACRIM-S4-016-2017) SiCO Anode Materials: DFT Simulations of Li Insertion

P. Kroll^{*1}; S. Haseen¹

1. UT Arlington, USA

We present combined modeling and simulation studies of Li insertion in amorphous SiCO ceramics to understand the high capacity of these novel anode materials. Atomistic models of amorphous SiCO in various forms, glasses with and without so-called "free" carbon, idealized SiO₂-C bilayer systems, and nano-structured SiCO models have been crafted and investigated within density functional theory. Random insertion of Li atoms tests for sites with high and favorable insertion energy. As shown previously, Li prefers bonding to O as cationic Li⁺, while the surplus electron is promoted to unoccupied state. Availability and locality of an electron reservoir determines enthalpy of insertion and charge distribution in the system. A fortuitous balance between Li-O bonding and electron promotion exists for aromatic carbon embedded in SiCO. When inserting multiple Li into SiCO we observe a strong correlation between the amount of Li possible to insert and the number of C atoms in aromatic segregations. This trend matches matches experimental observation. Thus, our computational studies provide fundamental understanding of the high Li capacity of SiCO compounds.

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(PACRIM-S4-017-2017) Flexible SiZrOC ultrafine fiber mat with enhanced high-temperature stability

Y. Wang^{*1}; J. Wang¹; H. Wang¹

1. National University of Defense and Technology, China

Despite tremendous efforts have been devoted to enhancing thermal stability of SiOC fibers, developing a simple and straightforward method to prepare SiZrOC ultrafine fibers still remains a challenge. Owing to easy processability, tailored composition and structure, polymer-derived ceramics (PDCs) route presents distinct advantages in preparing complicated silicon-based fibers. Herein, we provide a flexible zirconium modified silicon oxycarbide (SiZrOC) fiber mat via a simple electrospinning process combined with PDCs route. The spinning solution was prepared from a sol-gel system composed of zirconium n-butoxide and vinyltrimethoxysilane as raw materials, polyvinylpyrrolidone as the polymer for the fibers formation, acetic acid as a stabilizer and HNO₃ as a catalyst in water/alcohol solvent, separately. After reaching a suitable viscosity at ambient condition, the precursor solution was electrospun to be ultrafine fibers. Subsequent pyrolysis in nitrogen atmosphere turned the green fibers into SiZrOC ceramic fibers. Both the green fibers as well as the ceramic fibers were investigated by FTIR, XRD, SEM and TGA. The SiZrOC ultrafine fibers are relatively uniform with a diameter of 600-900 nm, without any noticeable flaws in the surface. The SiZrOC ultrafine fiber show good high temperature stability and flexibility. The residue weight at 1200 °C was 97.5 wt% for SiZrOC and 90.9 wt% for SiOC.

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(PACRIM-S4-018-2017) Promising attempts to get ultrathin boron nitride layers by Polymer Derived Ceramics

F. Gombault^{*1}; B. Toury¹; A. Brioude¹; C. Journet¹

1. Université de Lyon, Laboratoire des Multimatériaux et Interfaces, France

Polymer Derived Ceramics (PDC) route is an efficient method to synthesize ceramics with various shape such as monoliths and thin films. Starting from a monomer precursor, the polymerization process allows to adjust the chemical and physical properties