CHEMICAL SELF-ORGANIZATION SCALES OF ORDER IN NON-CRYSTALLINE AND NANOCRYSTALLINE ALLOYS

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Chemical bonding self-organizations that minimize macroscopic strain are crucial for performance of non-crystalline thin films in nano-scale CMOS devices. This presentation includes several new aspects of nano-scale thin film physics that are derived from electronic structure theory, and provide a way to obtain the inherent relationships between nano-scale strain-reducing chemical bonding selforganizations, and ultimate limits of device scaling. This issue is first addressed for non-crystalline (noc) SiO_2 and then for nanocrystalline (nano) transition metal gate dielectrics and other thin films.

There has been much debate relative to intermediate (medium) range order (I(M)O) in non-SiO_2 and (nano)-transition metal oxides proposed to extend device scaling into the deep sub-nm regime, and at the same time provide new chip functionalities. This presentation identifies the determinant role of symmetry controlled electronic structure in establishing two MRO scales of order that contribute to the position and full width half maximum, FWHM, of first sharp diffraction peak, FSDP, obtained from X-ray and neutron diffraction for non-SiO_2. Coherent length scales require a mechanism for constructive bond shortening, and the energy stabilization of symmetry-determined interactions between 2nd nearest and more distant neighbor atoms. In non-SiO_2 the availability of d-orbitals on Si atoms provides an intrinsic way through $p\pi$-$d\pi$ symmetry constraints to narrow 3rd and 4th neighbor Si-O, and O-O pair correlation distances by forcing symmetries of Si d-states of 2nd neighbor Si atoms to be strongly correlated by charge transfer through an intervening O-atom. This establishes a correlation length, R, of 0.4 to 0.5 nm, and fixes of the position of FSDP in the scattering function. A longer incoherent length scale, L, from the FWHM of the FSDP provides a measure of cluster formation in nano-regime of ~1 to 1.2 nm. Chemical bonding self-organizations minimize strain propagation and establish compliant internal incoherent Si interfaces with the non-SiO_2 films combined with interfacial transition regions with Si substrates and gate metals to limit the down-scaling of the physical thickness of gate dielectrics to 1.5 nm, consistent with experiments that extend to Si oxynitride alloys as well.

The capacitance equivalent thickness for nano-crystalline high-k gate dielectrics is defined by scaling with dielectric constant ratios, and thereby providing the ultimate fundamental limit for device scaling in the nano-scale ULSI regime. Once the physical thickness of a transition metal oxide, e.g., HfO_2, is reduced to < 2.5 nm, Jahn-Teller distortions are no longer possible, and thin films become X-ray amorphous with nano-grains having incoherent grain boundaries. This minimizes strain, and leads to reduced densities of defects. The presentation will also include other examples including Si nitride gate dielectrics for thin film transistors, and active and passive regions for rewritable optical memory materials.

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