Geochemical constrains and tectonic significance of Late Cretaceous mafic dykes from the Bhavani shear zone, South India

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South Indian Granulite Terrain (SIGT), a composite crustal unit, comprises multiply deformed litho-blocks dissected by crustal-scale shear zones with the history of multiple phases of reactivation. The Palaghat-Cauvery Shear System (PCSS), the prominent among these, is an Archaean crustal boundary with repeated reactivation and is believed to have an integral role in the modeling and reconstruction of Gondwana supercontinent. This terrain bears significant evidences of extensive magmatic activity in the form of dyke swarms, puncturing the granulites as well as the shear zone rocks. Mafic dyke swarms of varying composition and age are common in all the lithological units of the Palaghat-Cauvery Shear System (PCSS). The present study is an attempt to discuss the characteristic geochemical signatures and the tectonic background of the probably late Cretaceous mafic dykes which have important relations to the timing and tectonics of amalgamation of the Gondwana supercontinent. The mafic dykes, occurring at different parts of the Bhavani Shear Zone (BSZ), a constituent of the PCSS, are relatively fresh and have distinguishing structural relations and geochemistry. Geometrical analysis of joint patterns in these dykes suggest both predefined and self generated path for emplacement, the strain localised domains in the shear zone exerting a spatial control.

Geochemical studies indicate sub-alkaline tholeiitic basalt nature for these dykes with both high-Mg and high-Fe tholeiitic characters. Incompatible elements modeling suggests a depleted mantle source for these dykes and the average REE distribution in these dykes indicate considerable fractionation and possible crustal contamination as well as probable elemental mobility. Tectonic discriminations imply MORB characteristics as well as oceanic island affinity. Correlation of geochemical characteristics with other coeval units in the similar tectonic environments suggests an affinity to Marion Hotspot. In general comparison, these basalts are similar to the 45^0 E Indian Ocean ridge basalts and the basaltic rocks of eastern Madagascar volcanic province. The characteristic features of these dykes are discussed in terms of late Cretaceous Indian ocean tectonics and Gondwana reassembly.

Computational Study of Rutile and Quartz Interfaces with Aqueous Solutions

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In the past, we have obtained numerous simulation and experimental results of the TiO_2/aqueous solution interface including structure of adsorbed water and ions [1], hydrogen bonding and profiles of distance-dependent viscosity and diffusivity [2]. Here we will present our results on prediction of zeta potential (ζ) from molecular dynamics simulations and determination of dielectric properties of the interface. Our results show that the molecular nature of water and specific interactions of ions with the surface are key phenomena giving rise to the observed behavior.

In contrast to our works on TiO_2 and SnO_2 interfaces, our modelling of quartz (101) interface has been initiated only recently [3]. We have developed a model of negatively charged quartz, necessary for modeling of quartz surfaces above its point of zero charge ($pH_{pzc} \approx 2$-4.5), by a modification of the ClayFF force field [4], keeping the simple form of interaction potentials and introducing modified *ab initio* derived charges for a limited number of surface atom species. We present results of interactions of quartz (101) surface with aqueous solutions of NaCl and small organic molecules representing basic building blocks of larger biomolecules and functional groups of organic matter. As model molecules, benzoic acid, phenol, and salicylic acid were chosen. We studied interactions of molecules with surface for a set of surface charge densities 0.00, -0.03, -0.06 and -0.12 C/m^2, approximately corresponding to pH values 4.5, 7.5, 9.5 and 11.

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