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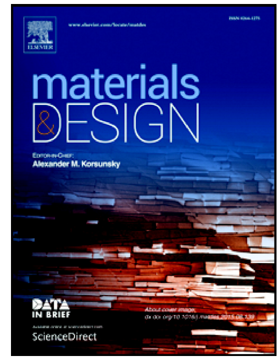

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Effects of antioxidant functionalized silica on reinforcement and anti-aging for solution-polymerized styrene butadiene rubber: experimental and molecular simulation study

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Abstract: A new type of antioxidant functionalized silica (SiO_2-g-MC) was prepared by grafting antioxidant N-(4-aniline phenyl) maleic imide (MC) onto the surface of silica via γ-mercaptopropyl trimethoxysilane (KH590). The effects of SiO_2-g-MC on reinforcement and anti-aging for solution-polymerized styrene butadiene rubber (SSBR) were investigated by experimental and molecular simulation methods. It was found that the reinforcement of SiO_2-g-MC was much more effective than that of the neat silica (SiO_2) in SSBR matrix due to well-dispersion and strong interfacial interaction between SiO_2-g-MC and SSBR. Compared with KH590 modified silica (SiO_2-KH590) and SiO_2, SiO_2-g-MC had better vulcanization behavior and could greatly improve thermo-oxidation resistance of SSBR composite. Furthermore, grafting MC onto the surface of silica could not only restrain the migration of free MC, but also reduce the negative influence of free MC on cross-linking density of SSBR composite. Therefore, SiO_2-g-MC/SSBR composite exhibited more preeminent mechanical properties than SiO_2-KH590/MC/SSBR composites during the thermo-oxidation aging process. These results indicated that SiO_2-g-MC could be used as a functional filler for the preparation of high performance SSBR composites, and moreover, the theoretical molecular simulation process can help us gain a better insight into the structure-property relationship for SSBR composite.

Key words: antioxidant functionalized silica, composite, reinforcement, anti-aging, molecular simulation

1. Introduction

As is known to all, diene rubber materials (such as natural rubber, styrene butadiene rubber, and butadiene rubber etc.) with a lot of isolated unsaturated carbon-carbon double bonds exhibit exceptional high elasticity and are irreplaceable in many industrial fields [1, 2]. But unfortunately, the instability of carbon-carbon double bonds and active allyl hydrogens in rubber molecular chain enables rubber materials to be vulnerable to aging when exposed to oxygen, ozone, light, heat and so on [3-5]. In particular, the thermo-oxidative aging, as one of the most common aging type, could dramatically deteriorate the physical or chemical properties of rubber materials and make rubber products premature failure, leading to a great waste of rubber resources in the word every year and even threatening the safety of human beings [6, 7]. Therefore, it is significantly important to prolong service life of rubber products by retarding their thermo-oxidative aging process.

At present, adding chemical antioxidants like derivatives of aromatic amine or phenol into rubber matrix is one of the most convenient methods to prevent rubber materials from the thermo-oxidative aging [8, 9]. These antioxidants could remarkably improve the thermo-oxidative stability of rubber, but usually, they are liable to migrate from rubber matrix because of low molecular weight, especially under conditions of low pressure, liquid, high temperature, etc.,