

Interrelations of Quantum-Mechanical Quantities Concerning Chemical Reactivity of Conjugated Molecules

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It is attempted to disclose the interrelations underlying the parallelism found in several quantum-mechanical methods previously proposed to explain chemical reactivity in conjugated molecules. This is carried out mathematically in alternant hydrocarbons and hetero-alternant molecules mainly by the use of Coulson's integral formulas. In an alternant hydrocarbon, provided a condition is satisfied between minors of the secular determinant, the orders of reactivity of each position predicted by the self-polarizability, free valence, superdelocalizability, Wheland's localization energy, and Dewar's approximate localization energy by NBMO are shown to be in complete agreement with one another. The relation of the frontier electron density and superdelocalizability is discussed. It is also demonstrated that a nonperturbation treatment for the so-called static method leads us to the same conclusion as the perturbation treatment. The parallelism of various quantities is discussed in their relation to the effect of heteroatom in heteroalternant molecules.

Electron Microscopic Studies on Fillers for Rubber. (IV)

State of Rubber-Filler System at the Elongation

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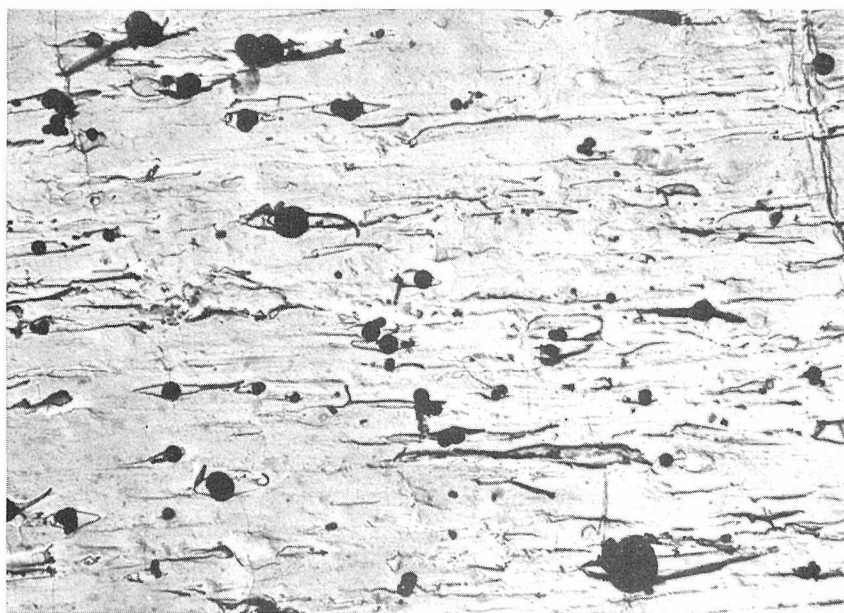
J. Soc. Rubber Ind., Japan, (Nippon Gomu Kyokaishi) **30**, 251 (1957)

The rubber samples loaded with various fillers were elongated 200, 400, 600% by Martens-Schopper machine respectively, and after two hours standing the samples were prepared by the methylmethacryl-SiO two-step casting replica method of electron microscopy. The film was prepared from sticky liquor obtained by dissolving polymethacryl in acetone. The liquor was spread over the surface of the sample, and after drying, it was removed from the surface. Swelling or any other changes due to the acetone solution were not recognized on the sample. After the Cr-shadowing, SiO was evaporated on this film, and then the original film was dissolved in the solvent.

Two kinds of carbon black (fine thermal type), three kinds of calcium carbonate, basic magnesium carbonate and clay were used as filler.

ABSTRACTS

In the electron micrographs of each samples at the time of elongation, many parallel streaks running to the tensile direction were observed, whereas they could not be observed in the unelongated original rubber. Cleavages were also observed clearly at both edges of filler particles at the tensile direction as shown in Fig. 1. At the time of elongation, it is conceivably possible that there grow cleavages at both edges of filler particles. The existense of the cleavages, which has already been speculated by Schippel (1920), was proved at the surface of rubber, and its shape was demonstrated.



Electron micrograph of the elongated rubber loaded with carbon black. Cleavages at both edges of filler particles are observed. Methethyl methacryl-SiO two-step casting replica was used. ($\times 16,000$)

A Specimen Preparation Technique for the Crystal Habit Analysis of Fibrous Crystals

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A simple technique is presented for the preparation of a specimen containing "rafts" of slender crystals to study the fiber period, growth direction, crystal habit, etc.

A small amount of specimen powder is ultrasonically dispersed in an organic medium which is not soluble in water and does not act as a solvent for the powder. A small quantity of suspension is floated on a surface of water. It spreads all over the surface and the needle-like crystals flow along local streaming