Chain-end effects in Su-Schrieffer-Heeger-type models of alternating trans-polyacetylene.
Foerner, Wolfgang

Abstract

Finite chain-length effects on soliton dynamics in Su-Schrieffer-Heeger models for trans-polyacetylene are reported and indicate that for the frequently used value of 0.1 .ANG. for the dimerization const., the results depend strongly on the chain length. An equation for the potential due to σ-electrons is reformulated so that no addnl. linear terms to avoid chain shrinkage are necessary. Second-neighbor resonance integrals of a magnitude suggested by exptl. findings had no influence on soliton dynamics.