**Dick B G, Jr. & Overhauser A W.** Theory of the dielectric constants of alkali halide crystals. *Phys. Rev.* **112**:90-103, 1958.
[Cornell University, Ithaca, NY]

This paper introduced the shell and exchange charge models designed to describe the interrelation of polarization and short-range interactions in solids. The models were applied to alkali halides so as to clarify the dielectric properties of these crystals. [The *SCI*® indicates that this paper has been cited in over 420 publications since 1958.]

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April 10, 1985

The frequent citation of this paper has probably been due to the simplicity and utility of the models developed and to the fact that the phenomena they describe are important. The shell model has become a standard tool in lattice dynamics following its application by Woods, Cochran, and Brockhouse to phonons in ionic crystals.[3] Since the publication of our paper, the shell model has been considerably generalized, put on a firmer theoretical basis, and used in many connections beyond those with which we were originally concerned.

This paper was based on a part of my PhD thesis research that I did under the direction of A.W. Overhauser at Cornell University between 1955 and 1957. Overhauser had suggested that I try to understand the physical reasons for the failure of the so-called Szigeti relations.[1,2] These are two equations relating experimental quantities for alkali-halide crystals that should be satisfied if the Born-Mayer model for these crystals were valid. They are not satisfied.

We decided to concentrate on the second of the Szigeti relations, the failure of which indicates a flaw in the account of dielectric phenomena given by the Born-Mayer theory. Szigeti had suggested that this failure might have something to do with polarization produced by short-range interaction forces. Using a simple Heitler-London treatment of the He-He short-range interaction, we managed to gain some simple insights into interactions between closed-shell atoms, and these led us to several extensions of the Born-Mayer model.

There were two models that seemed particularly promising that we called the "spring model" (later called the shell model) and the "exchange charge model." In the shell model, the ions are replaced by positively charged cores and rigid negatively charged spherical shells. Springs were imagined to provide a restoring force between shells and cores, and the repulsive forces between ions were modeled by springs between shells. The exchange charge model was intended to keep track of the charge redistributions that occur as a result of the requirements of the Pauli exclusion principle when ions begin to overlap. Both models might be termed simpleminded approaches to many-body effects. When incorporated in a theory of dielectric polarization, these models gave a plausible account of the failure of the second Szigeti relation and also clarified the idea of crystal polarizabilities of ions. We had a lot of fun arguing about and trying to justify these models to ourselves. The referee of our paper didn't like it very much and particularly objected to accounts of our efforts to justify the models. We persevered.

1. **Szigeti B.** Polarisability and dielectric constant of ionic crystals. *Trans. Faraday Soc.* **45**:155-66, 1949. (Cited 355 times since 1955.)
2. -------------. Compressibility and absorption frequency of ionic crystals. *Proc. Roy. Soc. London Ser. A* **204**:51-62, 1950. (Cited 210 times since 1955.)
3. **Woods A D B, Cochran W & Brockhouse B N.** Lattice dynamics of alkali halide crystals. *Phys. Rev.* **119**:980-99, 1960. [See also: **Woods A D B.** Citation Classic. *Current Contents/Engineering, Technology & Applied Sciences* **16**(16):18, 22 April 1985, and *Current Contents/Physical, Chemical & Earth Sciences* **25**(16):18, 22 April 1985.]

 