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Woods A D B, Cochran W & Brockhouse B N. Lattice dynamics of alkali halide crystals. *Phys. Rev.* 119:980-99, 1960.
[Physics Division, Atomic Energy of Canada Limited, Chalk River, Ontario, Canada]

This paper reported the first neutron-scattering measurements of phonon dispersion curves for a crystal containing more than one kind of atom, in this case sodium iodide The measurements were compared with calculations based on the then-developing shell model, which took into account the polarizability of the large negative ion in a particularly simple way The agreement between calculation and experiment provided support for the usefulness of the model [The *SCI*® indicates that this paper has been cited in over 395 publications since 1960]

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The alkali halides must be among the all-time favorites of physicists and chemists concerned with the properties of condensed matter, probably because their interatomic forces, dominated by electrostatic forces between ions, are thought to be better understood and more amenable to calculation than are those in other solids. Many scientists had devoted much effort to calculating the physical properties of alkali halides. Therefore, this first direct measurement of phonon dispersion curves in an alkali halide crystal was of considerable interest to a large constituency. This widespread interest in alkali halides was reflected in their being chosen for a major neutron-scattering study, at Chalk River Nuclear Laboratories, of their lattice dynamical properties. Sodium iodide was selected for the initial experiments because its large mass ratio ensured good separation of optic and acoustic modes, and its neutron properties, while not ideal, were acceptable.

A major attraction of this paper was its demonstration of the power of slow-neutron scattering (neutron spectroscopy) in getting direct information on interatomic forces in crystals. Bert Brockhouse, a coauthor, had successfully used the technique to study other systems, and his contributions to this field have led to many awards and honors including the Oliver E. Buckley Prize of the American Physical Society and fellowship in the Royal Society (London). He has also been made an Officer of the Order of Canada. It was a great privilege for me to work closely with him and to be able to participate in such an exciting research program.

Another reason for the attention this paper received was its contribution to the theory of the lattice dynamics of alkali halide crystals. My other coauthor was Bill Cochran, a crystallographer from Cambridge University who was spending a year at Chalk River. He recognized and convincingly demonstrated that the shell model of Dick and Overhauser[1] (a model that treated the static polarizability of ions in a particularly simple way) could overcome some of the deficiencies of earlier theoretical approaches to the lattice dynamics of alkali halides. I like to think that his subsequent election to fellowship in the Royal Society (London) was at least partly a result of this work at Chalk River. The interaction between the experimental and theoretical developments was exemplified during the course of this work when I was becoming frustrated by my inability to observe a certain zone-boundary mode. Feeling I had nothing to lose, I looked for—and found—the desired mode at a position in reciprocal space where it should have been unobservable. On the very morning I proudly displayed this result to my colleagues, Cochran informed me that it agreed with his new shell-model-based structure-factor calculations and that he was just about to suggest looking where I did. The shell model's popularity has been increasing ever since.

The experimental and theoretical work reported in this paper was later extended at Chalk River[2,3] and elsewhere The quoting of these newer results in the textbooks of the 1980s[4] is both a tribute to the contributions of neutron scattering to condensed-matter physics and a reminder of the continuing popularity of alkali halide crystals.

1 **Dick B G, Jr. & Overhauser A W.** Theory of the dielectric constants of alkali halide crystals *Phys Rev* 112 90-103, 1958 (Cited 445 times)
2 **Woods A D B, Brockhouse B N, Cowley R A & Cochran W.** Lattice dynamics of alkali halide crystals II Experimental studies of KBr and NaI *Phys Rev* 131 1025-9, 1963 (Cited 205 times)
3 **Cowley R A, Cochran W, Brockhouse B N & Woods A D B.** Lattice dynamics of alkali halide crystals III Theoretical *Phys Rev* 131 1030-9, 1963 (Cited 255 times)
4 **March N H & Parrinello M,** eds *Collective effects in solids and liquids* Bristol, England Hilger, 1982 274 p

