Table 1. *Orthosilicates: electronic polarizabilities of ions (in Å^3)*

Cation	α_{cation} (Pauling)	α_{cation} (Present paper)	$\alpha_{O^{2-}}$	Refinement
Be^{2+}	0·1	–	16·9	(*a*)
Mg^{2+}	1·2	0·1	19·8	(*b*)
Fe^{2+}	–	3·3	23·8	(*b*)
Zn^{2+}	3·6	5·4	21·8	(*c*)
Zr^{4+}	4·7	4·6	22·0	(*d*)

(*a*) Zachariasen (1971). (*b*) Birle, Gibbs, Moore & Smith (1968). (*c*) Klaska, Eck & Pohl (1978). (*d*) Robinson, Gibbs & Ribbe (1971).

Pauling's (1927) polarizabilities of Be^{2+}, Mg^{2+}, Zn^{2+} and Zr^{4+} are also given.

The agreement between the cation polarizabilities from Pauling's (1927) work and those from the present paper is passably close. For the polarizability of the O^{2-}, there is no value common to all orthosilicates.

When we first applied our calculations to willemite (Zn_2SiO_4), we used the structure refined by Chin'Hang, Simonov & Belov (1970). On the basis of this structure, however, we were unable to evaluate polarizabilities. For example, if we assumed reasonable values for the polarizabilities, the calculated birefringence was negative, while experimentally it was positive. On the other hand, we obtained the correct sign for the birefringence of phenacite (Be_2SiO_4), which is isostructural with willemite. Since the calculated refractive indices depend strongly on the shortest distances between highly polarizable ions, we doubted that the refinement of willemite had yielded accurate or nearly accurate coordinates. The rather unusual Si–O bond lengths determined by Chin'Hang, Simonov & Belov (1970) strengthened this doubt. Fortunately, a hydrothermally grown single crystal of willemite was available to us. We therefore decided to refine this structure for our use. The results of our refinement are given in a separate paper (Klaska, Eck & Pohl, 1978). The coordinates of the re-refinement allowed a superior calculation of the desired polarizabilities to be made. Thus, it has been shown that accurate coordinates are necessary to evaluate refractive indices from structural data. Conversely, in special cases calculation of optical properties can serve as a test for the accuracy of a structure refinement.

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High-flux micro-resonators for X- and γ-ray lasers.

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It is shown that a small single crystal may resonate at a wide range of X- and γ-ray frequencies. Such a resonator should produce roughly 10^{11} times greater radiative flux density per photon than previous designs.

A high-flux resonant cavity is an essential component of a successful continuous-wave X- or γ-ray laser. A number of such devices have been described by various authors (Bond, Duguay & Rentzepis, 1967; Cotterill, 1968; Deslattes, 1968; Kolpakov, Kuz'min & Ryaboy, 1970; Navasardyan, 1973). In each case the operation depends on a series of Bragg reflexions from large perfect crystals, and, in the main, these devices have planar or near-planar X-ray paths. Such a configuration suffers from a number of disadvantages, which may be listed as follows:

(1) It is difficult to design such a device with a resonant volume of less than a few tens of cubic millimetres. This implies relatively low radiative flux densities which in turn reduces the possibility of stimulated emission.

(2) Losses in the reflectors are additional to losses in the active medium and therefore represent an unnecessary inefficiency.

(3) Divergence of the beam at right angles to the diffraction plane is not unduly restricted; this leads to a progressive reduction in the radiative flux density.

(4) Multiple scattering is likely to be a severe source of loss, especially for almost symmetric crystals and short wavelengths; this appears to have been ignored in earlier work.

(5) The machining and precise alignment of large perfect crystals is not a trivial task.

Most of these problems may be overcome by generating

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X- or γ-rays within a small single crystal and localizing the photons by diffraction.

The localization process must obviously entail a situation where the probability of diffraction in any given direction is equal to the probability of diffraction in the reverse direction. This symmetry suggests that, in general, localization will occur when the reciprocal-lattice points touching the Ewald sphere are centrosymmetrically disposed about its centre. Pairs of centrosymmetrically related points will define diameters of the Ewald sphere which correspond to reflexions with $2\theta = \pi$. Such reflexions have already been studied theoretically by Kohra & Matsushita (1972) and, indeed, these authors recommend such reflexions for X-ray resonators because of the exceptionally broad total reflexion region.

Since each reciprocal-lattice vector will correspond to a resonance, the number of resonances associated with a specific crystal will be very large. The density of resonances per unit wavelength is given by differentiating with respect to the wavelength λ the expression for the number of reciprocal-lattice points contained by a sphere:

$$\frac{dN}{d\lambda} = \frac{-4\pi V}{\lambda^4 n_s},$$

where V is the volume of the primitive direct cell and n_s allows for the symmetry of the lattice. The density of resonances evidently increases very rapidly with decreasing wavelength.

As observed by Cotterill (1968), fine tuning is possible by allowing thermal expansion to vary the lattice parameter. Since most materials have an expansion coefficient of the order of parts in 10^5 $(°C)^{-1}$, tuning over a range of 0·1% is a practical possibility. This implies that for wavelengths less than 1 Å, most crystals will have an accessible resonance, irrespective of cell parameter or wavelength.

Thus, resonance within a small single crystal provides the properties of a macro-resonator, yet overcomes the associated problems, *i.e.*:

(1) The resonant volume for a single photon will be typically tenths of a cubic micron (see next section). This represents an improvement of the order of 10^{11} in radiative flux density per photon, which should be of substantial assistance in attaining stimulated emission.

(2) Reflexion losses are also active-medium losses. The X- or γ-ray mirrors are therefore effectively 100% efficient.

(3) Because $2\theta = \pi$, beam divergence in all directions perpendicular to the photon direction is fairly tightly controlled by diffraction processes.

(4) Multiple scattering will decrease the resonant volume and so will increase rather than reduce the radiative flux density.

(5) It is a simple matter to grow small single crystals of most materials. Because of the large width of the $2\theta = \pi$ reflexions, a small degree of imperfection will not unduly affect the resonator performance.

Micro-resonator performance

The $2\theta = \pi$ reflexion is virtually equivalent to two Bragg reflexions juxtaposed. Following the theory of Darwin (1914), therefore, there will be an exponential decrease in radiative flux density on either side of the point of origin of the resonant photon. The full-width at half-height of this flux distribution will be $5{\cdot}55q/\pi a$, where q is the reflecting power per crystal plane and a is the plane spacing. Typically, this will be of the order of tens of microns. Since there is a finite radiative flux density at the boundaries of the crystal, there must be a finite probability of radiation. The size and shape of the crystal may therefore be chosen to give the desired radiative coupling.

Kohra & Matsushita (1972) have shown that total reflexion widths of 0·2° are feasible with $2\theta = \pi$ reflexions. This implies that a resonant photon will be constrained to a cone of roughly 0·1° semi-angle. Calculations show that most K X-rays are likely to be reflected several times before absorption in their parent material. The lateral extent of a resonant photon is therefore likely to be less than 0·1 μm and the total resonant volume will be a few tenths of a cubic micron.

As observed elsewhere (Kangan, 1974; Andreev & Il'inski, 1976), the Borrmann effect may considerably extend the lifetime of a photon within the resonator.

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