Modulated Structure of an Intermediate Plagioclase. I. Model and Computation

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Two models of an intermediate plagioclase feldspar are proposed, based upon a modulated structure where the modulating wave is defined by both the occupation and the displacement of the Na/Ca sites. Both models consist of out-of-step domains. In one, the domains have an identical non-centrosymmetric structure but are of opposing chirality. In the other model, the domains are centrosymmetric and are related by a $c/2$ translation. The methods for refining the models by least squares are derived. In a companion paper, the refinement of a plagioclase with composition An_{55} is carried out and the results are discussed.

1. Introduction

In five earlier papers (Toman & Frueh, 1971, 1972, 1973*a*, *b*, *c*) henceforth referred to as TF1, TF2, TF3, TF4 and TF5 respectively, the X-ray diffraction studies of a sample of plagioclase with approximate composition An_{55} have been reported. In TF4 the Patterson functions based on intensities of *e* and *f* satellites were described; in TF5 the calculation of its 'average' structure based on *a* reflections was reported. For nomenclature of plagioclase reflections and atomic positions see Megaw (1956). The two present papers are mainly concerned with a least-squares calculation using *e* satellite intensities. All of the TF studies were based upon the same sample, described in detail in TF1 and TF2.

For the sake of convenience, the work presently reported has been divided into two parts. In the present paper, the general features of the modulated-structure model used in the computation are described. The companion paper describes the specific selections of models, and gives numerical results and a comparison of present results with published conclusions relative to other feldspar structures.

The present model is based on the concept of a modulated structure. This type of faulted structure was introduced into structural research many years ago and was applied mainly to certain types of alloys [see, for instance, Guinier (1963)].

The first attempt to treat the superstructure in intermediate plagioclase as a modulated structure was by Korekawa & Jagodzinski (1967). In that paper a qualitative explanation for the existence of satellites in the diffraction pattern of certain plagioclases was offered, using a modulated structure in which the occupation of the Na/Ca sites defined the modulating wave.

Unfortunately, that model does not adequately solve the problem of plagioclase satellites, because it ignores displacements of atoms from 'average' positions. These displacements, and not the substitutions, are the major contributors to the intensities of satellite reflections, as has been shown in TF1 and TF2. But, in spite of the fact that the Korekawa & Jagodzinski modulated-structure model fails to explain fully the superstructure of intermediate plagioclase, the modulated-structure idea appears very fruitful, especially if atomic displacements are included as well. This is the main subject of the two present papers.

2. Average structure

The starting point in a study of any superstructure is the determination of the average structure. Results of such a study for plagioclase An_{55} were presented in TF5, where the coordinates were given for 26 independent average sites in a 7Å subcell (referring to a subcell with *c* axis of ~ 7 Å), using the non-centrosymmetric space group $C1$. The calculation was based on a standard least-squares method (720 reflections; 115 parameters; and an *R* value of 0·097 in semi-anisotropic approximation).

Fortunately, it was later discovered that the *R* value can be considerably lowered by accepting the fact that the average structure is faulted, and basing the calculations on the apparent centrosymmetric space group $C\bar{1}$ while maintaining 26 sites now considered as occupied by half-atoms (720 reflections; 115 parameters; and an *R* value of 0·072 in semi-anisotropic approximation). In this calculation only the Na/Ca sites are treated anisotropically. The resulting atomic coordinates are very similar to those obtained for the $C1$ case.*

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* A table of atomic positions and isotropic temperature coefficients of: (1) unfaulted non-centrosymmetric average structure, refinement using equation (1); (2) faulted structure, apparent space group $C\bar{1}$, refinement using equation (1); and (3) faulted structure, apparent space group $C\bar{1}$, refinement using equation (2); as well as a table of the anisotropic temperature coefficients β_{ij} for the Na/Ca sites are deposited with the British Library Lending Division as Supplementary Publication No. SUP 31250 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

The fact that the agreement improved substantially after half-atoms were introduced, without increasing the number of adjustable parameters, is very important because it indicates that the averaging by which the average structure was obtained involves not only averaging over atomic positions displaced by modulating waves but also averaging over out-of-step domains.

Furthermore, in accepting the idea of a modulated structure, it is necessary to realize that the structure factors of average reflections expressed by

$$F_{hkl} = \sum f_j \exp\left[2\pi i(hx_j + ky_j + lz_j)\right] \qquad (1)$$

is only a first approximation [see, for instance, Wilson (1962)]. Therefore, the refinement of the a reflections by using standard least-squares routines is only approximately valid. For more exact calculations it is necessary to use a least-squares routine based on

$$F_{hkl} = \sum \psi_j \exp\left[2\pi i(hx_j + ky_j + lz_j)\right] \qquad (2)$$

where ψ_j is a generalized structure factor containing amplitudes of modulating displacement and substitution waves (see Appendix). Unfortunately, these amplitudes are not available at the beginning, and therefore this calculation can be attempted only after displacements have been determined from calculations based on satellite reflections. For this reason, coordinates of half-atoms calculated using formula (2) are included in Table 1 of the following paper. The R value obtained for this refinement is 0·071, but the number of parameters is only 82 because only three isotropic temperature factors are used in the program (one for each type of atom).

As can be seen from Table 1 in the accompanying paper, only Na/Ca sites and a few other sites have differences in half-atom positions large enough to exceed errors by a reasonable margin. Therefore, for most atoms their average positions in both out-of-step domains are identical; if in spite of this fact the structure is treated as if composed of two out-of-step domains with respect to all atoms, it is treated thus only for the sake of uniformity in the computation.

3. Modulated structure

As has already been stated, the model on which the present calculations of the plagioclase superstructure are based is a model of a modulated structure. In this model the atoms are displaced from their average positions by displacements determined by a modulation wave running through the structure. Each of the 26 independent positions in the subcell is associated with a modulation wave of the form

$$\Delta_{1j} \cos 2\pi(\mathbf{r} \cdot \mathbf{B}_T + {}_{\Delta}\varphi_{1j}) + \Delta_{2j} \cos 4\pi(\mathbf{r} \cdot \mathbf{B}_T + {}_{\Delta}\varphi_{2j}); \qquad (3)$$

here, $\mathbf{r}$ is a position vector of a point for which (3) described its displacement; $\mathbf{B}_T$ is the wave vector of the modulation wave; Δ_{1j} is the amplitude of displacement of the e component of the modulation wave; ${}_{\Delta}\varphi_{1j}$ is its phase; and Δ_{2j} is the amplitude of displace-

ment associated with the f component of the modulation wave and ${}_{\Delta}\varphi_{2j}$ is its phase. Wave vector $\mathbf{B}_T$ is constant for all modulation waves and its value can be determined from the separation of pairs of satellite reflections in reciprocal space; therefore, it is a parameter readily obtainable by experiment. As there are two types of satellites (e and f), there are two components of the modulation wave: the e component, with wavelength $1/B_T$, characterized by Δ_{1j} and ${}_{\Delta}\varphi_{1j}$, mainly responsible for the e satellites; and the f component, with wavelength $1/2B_T$, characterized by Δ_{2j} and ${}_{\Delta}\varphi_{2j}$ and mainly responsible for the f satellites. For details see Appendix.

In the anorthite unit cell there are 104 atomic sites having positions which can be approximately or exactly derived from 13 sites by translations of $\mathbf{c}/2$, $(\mathbf{a}+\mathbf{b})/2$, $(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$ and the operation of the inversion center.

On the diffraction picture of a plagioclase, e satellites are centered on reciprocal lattice points (anorthite cell) with $h+k=2n+1$, $l=2m+1$ (b points), and f satellites are centered on reciprocal lattice points with $h+k=2n$, $l=2m$ (a points). Otherwise they are absent. To satisfy these conditions, Korekawa & Jagodzinski (1967) proposed in their modulated-structure model that e components of modulation waves corresponding to atoms related by translations $\mathbf{c}/2$ or $(\mathbf{a}+\mathbf{b})/2$ have phase difference π, but that e components of modulation waves associated with atoms related by translations $(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$ are in phase. For f components they postulate that all waves associated with sites related by translations $\mathbf{c}/2$, $(\mathbf{a}+\mathbf{b})/2$ or $(\mathbf{a}+\mathbf{b}+\mathbf{c})/2$ are in phase. These phase relationships are retained in the present model.

Similarly, as displacements of atoms from average positions are controlled by modulation waves, so are the occupations of the atomic sites. In the present work, only the occupations of the Na/Ca sites are considered as subjected to modulation. Obviously, there is no reason to expect that the occupancies of T sites are not modulated, but to introduce them into the model would be of little value because of the small differences in atomic scattering factors of Al and Si atoms.

The modulation waves describing the dependence of the atomic scattering factor of the jth atom site is of the form

$$f_j[1 + \varepsilon_{1j} \cos 2\pi(\mathbf{r} \cdot \mathbf{B}_T + {}_{\varepsilon}\varphi_{1j})$$
$$+ \varepsilon_{2j} \cos 4\pi(\mathbf{r} \cdot \mathbf{B}_T + {}_{\varepsilon}\varphi_{2j})]; \qquad (4)$$

here, coefficients ε_{1j} and ε_{2j} describe the change of atomic scattering factor due to the effect of the e and f components of the modulation waves; ${}_{\varepsilon}\varphi_{1j}$ and ${}_{\varepsilon}\varphi_{2j}$ are corresponding phases and f_j is the average atomic scattering factor.

The contribution from each atomic site to the structure factor of a satellite reflection is of the form:

$${}^t\psi_j \exp\left[2\pi i(x_j h + y_j k + z_j l)\right], \qquad (5)$$

where ${}^t\psi_j$ is the generalized atomic scattering factor corresponding to a reflection of the tth kind (1 for e,

2 for f satellites). A detailed discussion of the generalized atomic scattering factor is deferred to the Appendix.

4. Domain structure

As has already been mentioned in §2, the average structure of this plagioclase sample can best be described in terms of half-atoms, which implies that 'out-of-step' domains are present.

The observed average structure as it was computed from a reflections can result from either of two possibilities:

(i) The structure of each domain is non-centrosymmetric $(C1)$, the observed apparent symmetry $(C\bar{1})$ being obtained by superposition of identical domains differing only in their chirality (left-handed or right-handed domains related by inversion).

(ii) The structure of each domain is centrosymmetric $(C\bar{1})$, the domains being related by translations, as in the case of bytownite (Fleet, Chandrasekhar & Megaw, 1966).

The second case might seem more likely, but it is necessary to realize that in a modulated structure no true center of symmetry is presented. The inversion centers present in unperturbed structures lose their 'influence' over a long distance when modulation is applied to atomic sites. This circumstance makes the first case worth considering (for more details see Appendix in companion paper).

(i) The non-centrosymmetric case

Here, the structure consists of domains of identical structure but of opposing chirality. Each domain consists of 14Å unit cells containing 104 atoms. Only 26 sites in the unit cells are independent (those in Table 1); the remaining sites are derived by translations of $c/2$, $(a+b)/2$ and $(a+b+c)/2$. To obtain the observed apparent symmetry $(C\bar{1})$, left-and right-handed domains are present in equal proportion and the whole assembly diffracts coherently. Each site in a unit cell is associated with a modulation wave described by amplitudes Δ_{1j} and Δ_{2j} and phases $_{\Delta}\varphi_{1j}$ and $_{\Delta}\varphi_{2j}$. Furthermore, the Na/Ca sites are associated with a substitution modulation characterized by ε_{1j}, ε_{2j}, $_{\varepsilon}\varphi_{1j}$ and $_{\varepsilon}\varphi_{2j}$.

As can be deduced from the remarkable sharpness of e-satellite reflections observed on diffraction photographs of the sample, e modulation waves must be coherent over large distances. This implies that one modulation wave passes through several domains; across each domain boundary a phase change $\pm\alpha_j$ is expected, so that the phase of a modulation wave corresponding to site j is φ_j in domains of one chirality and $\varphi_j+\alpha_j$ in domains of opposite chirality.

The final contribution of the jth atom to the structure factor is

$$^t\psi_j[1+\exp(\pi i\alpha_j)]\cos 2\pi(x_jh+y_jk+z_jl)$$
$$+^t\psi'_j[1-\exp(\pi i\alpha_j)]\sin 2\pi(x_jh+y_jk+z_jl)\,. \quad (6)$$

(ii) The centrosymmetric case

Here, the structure of a domain consists of 13 sites with their centrosymmetrical counterparts, plus another 13 atoms translated with their centrosymmetrical counterparts by $c/2$. This arrangement has close similarity to the structure of bytownite. To satisfy the extinction rules for satellite reflections, it is necessary to have an out-of-step domain related by a $c/2$ translation and having a π phase change of the e components of the modulation waves (f components do not change phase).

As has been indicated before, true centrosymmetry does not exist in a modulated structure. It is impossible to expect identical modulation waves associated with an atomic site and its centrosymmetrical counterpart (centrosymmetry applies here only to average positions). For this reason, a phase difference α_j between two modulation waves of two centrosymmetrically related jth atoms is expected.

For the contribution of the jth atom to the structure factor, the same expression is obtained as in (6), but the meaning of α_j is different.

5. Least-squares calculation

For the study of different models of plagioclase superstructure, a number of least-squares programs were prepared:

(i) Refinement of the coordinates of the positions of 'average' atoms. As already stated, the starting approximation is the standard refinement technique based on equation (1), where displacements that are related to modulation waves are considered to be absorbed in temperature factors. After more is known about displacement and substitutional waves in the modulated structure, a least-squares program based on equation (2) is useful. The calculation is based on intensities of the a reflections; variable parameters optimized in the process as coordinates of average atomic sites, three isotropic temperature factors (for A, T and O atoms), and a scale factor. Input consists of atomic scattering factors, intensities and indices of a reflections, approximate coordinates of average atoms, modulation parameters Δ_{1j},Δ_{2j} for all sites, and, in addition, ε_{1j} and ε_{2j} for the Na/Ca sites. During the refinement, parameters of the modulation waves are held constant.

(ii) Refinement of the parameters of e components of the modulation waves. The calculation is based on e-satellite intensities. Variable parameters adjusted in the process are only Δ_{1j}, $_{\Delta}\varphi_{1j}$ and α_j for all atoms and, in addition, ε_{1j} and $_{\varepsilon}\varphi_{1j}$ for the Na/Ca positions. Input consists of average coordinates of the atomic scattering factors, temperature factors, approximate parameters of e and f modulation waves and components of the wave vector $\mathbf{B}_T$. All parameters except parameters describing the e component $(\Delta_{1j}, _{\Delta}\varphi_{1j}, \alpha_j, \varepsilon_{1j}$ and $_{\varepsilon}\varphi_{1j})$ are held constant. For initial runs, parameters of the f component may be neglected because the e-satellite intensities depend mainly on e modulation waves.

(iii) Refinement of the parameters of f components

of the modulation waves. The calculation is based on f satellites. Variables to be adjusted here are Δ_{2j} and $_{\Delta}\varphi_{2j}$ and, in addition, ε_{2j} and $_{\varepsilon}\varphi_{2j}$ for the Na/Ca sites. Input consists of intensities and indices of f satellites, atomic scattering factors, temperature coefficients, approximate parameters of the e and f components of the modulation waves, coordinates of 'average' atomic sites and components of the wave vector of the f component. All parameters except those describing the f component of the modulation waves (Δ_{2j}, $_{\Delta}\varphi_{2j}$, ε_{2j} and $_{\varepsilon}\varphi_{2j}$) are held constant. In initial runs, parameters of the e component may be neglected, because structure factors of f satellites depend mainly on f waves and, to a much lesser extent, on e waves (see Appendix). Calculation is of the block-diagonal type, each atom being treated independently.

The program for the refinement of the e-components of the modulation waves was used in the computations performed on the measured structure factors of e-satellite reflections (sample of composition An_{55}). The program for refinement of f-components of the modulation waves was used in the calculations executed on the measured structure factors of the f-satellite reflections. In both cases the calculation was performed using both the unfaulted non-centrosymmetric model and the faulted (domain structure) model in apparent space group $C\bar{1}$.

After completion of these calculations, the program for the refinement of positions of atoms in the 'average' structure was used in the calculations performed on the structure factors of the a reflections. Details of the refinement and a discussion of the results are contained in the companion paper immediately following.

APPENDIX

In TF3 the generalized atomic scattering of the jth site was defined as:

$$^t\psi_j = \frac{f_j}{N} \sum_{s=1}^{s=N} (1 + \varepsilon_{js}) \exp(2\pi i \Delta_{js} \cdot \mathbf{B}_H^t)\varphi_s^t, \qquad (7)$$

where N is the number of subcells in a supercell; f_j is the average atomic scattering factor of the jth site; ε_{js} is the increment of the atomic scattering factor of the jth site in the sth subcell; Δ_{js} is the displacement of the jth site in the sth subcell from its average position; $\beta_H^t = \mathbf{B}^t + \mathbf{B}_H$; and $\varphi_s^t = \exp(2\pi i \mathbf{r}_s \cdot \beta^t)$. Here, $\mathbf{B}_H^t$ is the reciprocal vector of a reflection of the tth kind (e-satellite and f-satellite) and $\mathbf{B}_H$ is the reciprocal vector of a main reflection close to the satellite reflection under consideration. Vector $\mathbf{r}_s$ is the position vector of the sth subcell.

In the special case of a modulated structure in plagioclase, when occupation and displacement of atomic sites are controlled by both components of the modulation waves (the e component and the f component),

equation (7) becomes:

$$^t\psi_j = \frac{f_j}{N} \sum_{s=1}^{s=N} [1 + \varepsilon_{1j} \cos 2\pi(\mathbf{r}_s \cdot \mathbf{B}_T + _{\varepsilon}\varphi_{1j})$$
$$+ \varepsilon_{2j} \cos 4\pi(\mathbf{r}_s \cdot \mathbf{B}_T + _{\varepsilon}\varphi_{2j})]$$
$$\times \exp\{2\pi i[\Delta_{1j} \cdot \mathbf{B}_H \cos 2\pi(\mathbf{r}_s \cdot \mathbf{B}_T + _{\Delta}\varphi_{1j})$$
$$+ \Delta_{2j} \cdot \mathbf{B}_H \cos 4\pi(\mathbf{r}_s \cdot \mathbf{B}_T + _{\Delta}\varphi_{2j})]\}$$
$$\times \exp[2\pi i t\mathbf{r}_s \cdot \mathbf{B}_T] . \qquad (8)$$

where $t = 0, 1, 2$ for a reflections, e satellites and f satellites.

By expanding the exponential function in powers of the scalar product of the displacement and reciprocal vectors, and by applying the binomial theorem and replacing cosines with an exponential function, we obtain

$$^t\psi_j = \frac{f_j}{N} \sum_{s=1}^{s=N} \exp(2\pi i t\mathbf{r}_s \cdot \mathbf{B}_T)\{1 + (\varepsilon_{1j} \exp[2\pi i(\mathbf{r}_s \cdot \mathbf{B}_T$$
$$+ _{\varepsilon}\varphi_{1j})] + \varepsilon_{2j} \exp[4\pi i(\mathbf{r}_s \cdot \mathbf{B}_T + _{\varepsilon}\varphi_{2j})] + \varepsilon_{1j}$$
$$\times \exp[-2\pi i(\mathbf{r}_s \cdot \mathbf{B}_T + _{\varepsilon}\varphi_{1j})] + \varepsilon_{2j} \exp[-4\pi i(\mathbf{r}_s \cdot \mathbf{B}_T$$
$$+ _{\varepsilon}\varphi_{2j})])/2\} \sum_{n=0}^{\infty} \frac{(iD_{1j})^n}{n!} \sum_{p=0}^{p=n} \binom{n}{p} \exp[2\pi i(\mathbf{r}_s \cdot \mathbf{B}_T$$
$$+ _{\Delta}\varphi_{1j})(2p-n)] \sum_{m=0}^{\infty} \frac{(iD_{2j})^m}{m!} \sum_{q=0}^{q=m} \binom{m}{q} \exp[4\pi i$$
$$\times (\mathbf{r}_s \cdot \mathbf{B}_T + _{\Delta}\varphi_{2j})(2q-m)] , \qquad (9)$$

where $D_{1j} = \pi\Delta_{1j} \cdot \mathbf{B}_H$ and $D_{2j} = \pi\Delta_{2j} \cdot \mathbf{B}_H$.

Now $^t\psi_j$ can be expressed as a sum of five terms:

$$^t\psi_j = {}^tA_{0j} + {}^tA_{1j} + {}^tA_{2j} + {}^tA_{3j} + {}^tA_{4j}$$

where the first term does not depend on substitution modulation; the second and the third depend on the e component of the substitution modulation wave; and the fourth and fifth depend on the f-component of the substitution modulation wave (all terms dependent upon the displacement modulation).

For $^tA_{0j}$ we have:

$$^tA_{0j} = \frac{f_j}{N} \sum_{s=1}^{s=n} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \sum_{p=0}^{p=n} \sum_{q=0}^{q=m} \frac{(iD_{1j})^n(iD_{1j})^m}{n!m!} \binom{n}{p}\binom{m}{q}$$
$$\times \exp[2\pi i_{\Delta}\varphi_{1j}(2p-n)] \exp[4\pi i_{\Delta}\varphi_{2j}(2q-n)]$$
$$\times \exp[2\pi i(t + 2p - n + 4q - 2m)\mathbf{r}_s \cdot \mathbf{B}_T] . \qquad (10)$$

A summation over s eliminates all terms where $t + 2p - n + 4q - 2m \neq 0$; furthermore, using identity

$$i^p J_p(2\xi) = \sum_{t=0}^{\infty} \frac{(i\xi)^{t+p}}{(t/2)!(p+t/2)!} ,$$

$$^tA_{0j} = f_j \sum_{m=0}^{\infty} \sum_{q=0}^{q=m} \frac{(iD_{2j})^m}{q!(m-q)!} \exp[-2\pi i(2q-m)\delta_j]$$
$$\times \exp(-2\pi i t_{\Delta}\varphi_{1j}) \exp\left(\frac{\pi}{2}|4q-2m+t|\right)$$
$$\times J_{|4q-2m+t|}(2D_{1j}) \qquad (11)$$

where $\delta_j = 2(_\Delta\varphi_{1j} - _\Delta\varphi_{2j})$ and $J_p(2\xi)$ is a Bessel function of the first kind and of the pth order. Similarly, for the second and third terms $^tA_{1,2j}$ is obtained by using the same procedure:

$$^tA_{1,2j} = \frac{\varepsilon_{1j}}{2} f_j \sum_{m=0}^{\infty} \sum_{q=0}^{q=m} \frac{(iD_{2j})^m}{q!(m-q)!}$$

$$\times \exp\left[-2\pi i(2q-m)\delta_j\right] \exp\left[-2\pi i(t\pm 1)_\Delta\varphi_{1j}\right]$$

$$\times \exp\left(\pm 2\pi i_\varepsilon\varphi_{1j}\right) \exp\left[\frac{\pi}{2}|4q-2m+(t\pm 1)|\right]$$

$$\times J_{|4q-2m+(t\pm 1)|}(2D_{1j}) \tag{12}$$

and for the fourth and fifth terms:

$$^tA_{3,4j} = \frac{\varepsilon_{2j}}{2} f_j \sum_{m=0}^{\infty} \sum_{q=0}^{q=m} \frac{(iD_{2j})^m}{q!(m-q)!}$$

$$\times \exp\left[-2\pi i(2q-m)\delta_j\right]\exp\left[-2\pi i(t\pm 2)_\Delta\varphi_{2j}\right]$$

$$\times \exp\left(\pm 4\pi i_\varepsilon\varphi_{2j}\right)\exp\left[\frac{\pi}{2}|4q-2m+(t\pm 2)|\right]$$

$$\times J_{|4q-2m+(t\pm 2)|}(2D_{2j}) . \tag{13}$$

It is important to realize that in the first approximation

$$^0A_{0j} = f_j,$$

$$^1A_{0j} = if_j D_{1j} \exp\left(-2\pi i_\Delta\varphi_{1j}\right),$$

$$^2A_{0j} = if_j D_{2j} \exp\left(-4\pi i_\Delta\varphi_{2j}\right),$$

$$^1A_{2j} = \frac{\varepsilon_{1j}}{2} f_j \exp\left(-2\pi i_\varepsilon\varphi_{1j}\right),$$

$$^2A_{4j} = \frac{\varepsilon_{2j}}{2} f_j \exp\left(-4\pi i_\varepsilon\varphi_{2j}\right).$$

It follows from these expressions that e-satellite intensities are determined mainly by e components (D_{1j} and $_\Delta\varphi_{1j}$), whereas f components contribute higher-order corrections only. On the other hand, intensities of f satellites are determined mainly by f components (D_{2j} and $_\Delta\varphi_{2j}$), whereas parameters of the e waves are of minor importance here.

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