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On the core width and Peierls stress of bubble rafts dislocations within the framework of modified Peierls-Nabarro model

Research Article

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Abstract: Using Foreman's method, the core structure and Peierls stress of dislocations in bubble rafts have been investigated within the framework of the modified Peierls-Nabarro (P-N) model in which the discrete lattice effect is taken into account. The core width obtained from the modified P-N model is much wider than that from the P-N model owing to the discrete lattice effect. It is found that the core width of dislocation increases with a decrease of the bubble radius. The elastic strain energy associated with the discrete effect is considered while calculating the Peierls stress. The new expression of the Peierls stress obtained in this paper is not explicitly dependent on the particular form of the restoring force law, which is only related to the core structure parameter and can be used expediently to predict the Peierls stress of dislocations. The Peierls stress decreases rapidly with the decrease of the bubble radius.

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Keywords: bubble rafts • dislocation • core structure

1. Introduction

Bubble rafts, a single layer of bubbles freely floating on a surface of water, have been widely used to exhibit topological defects such as dislocations, disclinations and grain boundaries, with vivid images of the structure of defects since first being introduced by Bragg and Nye to model metallic crystalline structures [1–4]. Bubble rafts have also been used to study nanoindentation of an initially defect-free crystal and dynamic behavior of crystals under shear [5, 6]. To date, the core width and Peierls stress of dislocations in bubble rafts have remained unsolved. In order to clarify the core structure of dislocations in bubble rafts, one should point out three problems appearing in the analysis of the dislocations core structure and Peierls stress within the scope of the dislocation lattice theory: (i) how to get the relation between restoring force law and radius of bubble rafts, (ii) what is the form of an unified dislocation equation for bubble rafts and (iii) the mainly mathematical problem related to the solution of the nonlinear dislocation equation. Foreman et al. proposed a phenomenological method for the more general case to remedy the defects of the sinusoidal force law in the framework of the Peierls-Nabarro (P-N) model [7].

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Based on the conclusions of Nicolson et al., Guo et al. obtain the relation between the restoring force law and the bubbles radius within the Peierls cut-glue scheme [8–11]. As is well known, the P-N model can predict the core width and Peierls stress of dislocations analytically [12–16]. However, the fundamental dislocation equation in the P-N model is derived from the balance between the nonlinear interaction from the misfit gluing and the linear interaction form the deformation, which is obtained by the assumption that the crystal is taken to be elastic continuum. Recently, a modified P-N dislocation equation taking into account the discrete lattice effect is presented on the basis of lattice statics and symmetry principles, which is important for the dislocation core structure [17–19].
Today, the remaining key task to determine the dislocation core structure is to obtain the solution of the modified P-N dislocation equation combined with the restoring force law for bubble rafts. An analytical expression of the force law for bubble rafts with different radii is presented in Ref. [8]. Unfortunately, the expression is so complex that attempts to solve the modified P-N dislocation equation are unsuccessful. In this paper, Foreman's method, an elegant idea for dealing with dislocation width with good generalization for different dislocations with different geometrical characters, is applied to find the solution of the modified P-N dislocation for bubble rafts [7, 13, 14]. The core widths obtained by P-N and modified P-N dislocation equation for bubble rafts with different radii are presented. The new expression of the Peierls stress obtained in this paper is not explicitly dependent on the particular form of the restoring force law, which is only related to the core structure parameter and can be used expediently to predict the Peierls stress of dislocations.

2. Core width of dislocations in bubble rafts

The modified P-N dislocation equation including the discrete lattice effect was obtained firstly by using the solvable models and secondly derived in a model-independent way, and takes the following form [17–19]

$$-\frac{\beta}{2}\frac{d^2u}{dx^2}-\frac{\mu}{2\pi(1-\nu)}\int_{-\infty}^{+\infty}\frac{dx'}{x'-x}\left(\frac{du}{dx}\right)\bigg|_{x=x'}=f(u), \tag{1}$$

where $u(x)$ is the relative displacement of the bilateral misfit planes along the glide direction. μ and ν are the shear modulus and Poisson's ratio, respectively. There is an extra second-order derivative in the modified P-N equation compared with the classical P-N equation, which denotes the modification of lattice discrete effect. β is the modification parameter of the discrete effect originated from the special structure of crystals. Generally, the bubbles are close-packed structure and the form of packing is taken to be two-dimensional triangular lattice. For a two-dimensional triangular lattice, the modified parameter $\beta=\frac{3}{4}$, shear modulus $\mu=\frac{\sqrt{3}}{4}$ and Poisson's ratio $\nu=\frac{1}{4}$ [17, 18]. $f(u)$ is the restoring foce law due to the atoms in the opposite glide plane, which can be obtained from the gradient of the generalized stacking fault (GSF) energy for materials $f(u)=-\frac{\partial\gamma(u)}{\partial u}$ [13, 14]. However, the GSF energy of bubble rafts is hard to obtain and the restoring force law for different radii is derived directly based on the interaction between bubbles within the Peierls cut-glue scheme [8]. As described above, the expression for the restoring force law for bubble rafts is complex and the dislocation equation cannot be solved by variational method, although it is an effective method to solve the integro-differential dislocation equation [20, 21]. In this paper, Foreman's method is applied to solve the modified P-N dislocation equation to determine the dislocation core structure in bubble rafts. Foreman's method is also be generalized to solve the dissociated and mixed dislocations by Medvedeva et al. [13, 14]. Foreman's solution for dislocations is typically given as follows [7, 22]

$$u(x)=\frac{b}{\pi}\left\{1-(\eta-1)\frac{\partial}{\partial\eta}\right\}\arctan\frac{p_0}{\eta}, \tag{2}$$

where $p_0=\kappa_0 x$ with $\kappa_0=\frac{2(1-\nu)}{d}$, which originated from the exact arctan-type solution of the P-N dislocation equation with the sinusoidal force law. η is an arbitrary parameter and $\eta=1$ corresponds to the solution for the classical P-N dislocation with a sinusoidal force law [23]. The core structure parameter η contains two modifications to dislocation core: the first results from the discrete lattice effect and the other is from the modification of the sinusoidal force law. The core width of dislocation is determined by the core structure parameter η and increases with the increasing of the core structure parameter.
Let $p_0=\eta\cot\left(\frac{\theta}{2}\right)$, the stress and displacements can be written in the convenient parametric form

$$\begin{aligned}\frac{2\pi d}{\mu b}\sigma=&\frac{8\beta b(1-\nu)^2\cot\left(\frac{\theta}{2}\right)\left(-3+4\eta+\cot\left(\frac{\theta}{2}\right)^2\right)}{\mu d\eta^3\left(1+\cot\left(\frac{\theta}{2}\right)^2\right)^3}\\&+\frac{2\cot\left(\frac{\theta}{2}\right)\left(-2+4\eta+\cot\left(\frac{\theta}{2}\right)^2\right)}{\eta^2\left(1+\cot\left(\frac{\theta}{2}\right)^2\right)^2},\end{aligned} \tag{3}$$

$$\frac{1}{b}u=\frac{1}{\pi}\left(\frac{\pi}{2}-\frac{\theta}{2}+\frac{\eta-1}{2\eta}\sin\theta\right). \tag{4}$$

The shear stress σ corresponding to the left of Eq. (1) are illustrated in Fig. 1 for $\eta=1,2,4,10$ within the framework of the P-N and modified P-N models. As can be seen, the maximum of the shear stress σ decreases as the core structure parameter η is increased, whereas the position of the maximum shear stress is increases. Furthermore, the maximum shear stress obtained in the modified P-N dislocation equation is larger than that of the P-N dislocation equation for the same core structure parameter η. This indicates that the same shear stress corresponding to the different core structure parameters η, and the core structure parameter is smaller in the P-N theory than that in the modified P-N theory. This indicates that the same shear stress corresponding to the different core structure parameters η, and η is smaller in the P-N theory than that in the modified P-N theory.

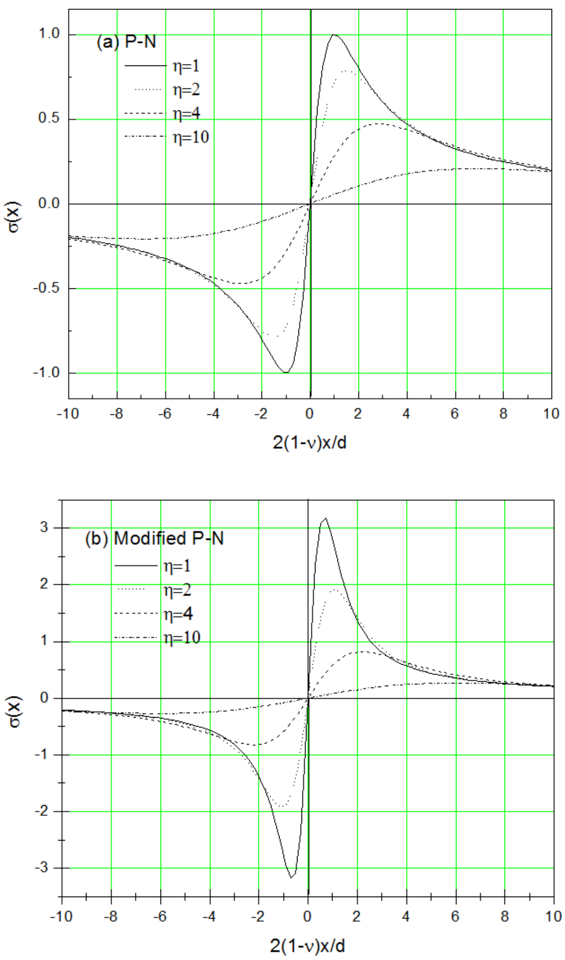

Figure 1. Shear stress distribution along slip direction: (a) the P-N theory, (b) the modified P-N theory.

The shear stress distribution along slip direction can be determined by atomistic simulation for crystals, and the core structure parameter η which controls the dislocation core structure is easily fixed [24]. Nowadays, the restoring force law is the only exist condition for the bubble rafts. According to Eq. (3) and Eq. (4), the relation between shear stress σ and the displacement u can be established. By comparing the $\sigma(u)$ with the restoring force law obtained in Ref. [8] for bubble rafts with different radii, the core structure parameters η can be obtained. The criterion of comparison is that both distributions have the same maximum shear stress $\sigma_{\max}$. This requirement is easily understood. The dislocation core width is mainly controlled by the maximum of the stable stacking fault energy (namely the unstable stacking fault energy), and the maximum of the shear stress has the same effect as the unstable stacking fault energy while describing the dislocation structure [20]. The results are listed in Tab. 1 for bubble rafts with different radii. The core structure parameter η obtained in the modified P-N theory is larger than that of the P-N theory, namely the dislocation core width is wider within modified P-N theory when the discrete lattice effect is taken into account. Although the maximum shear stress is increases with increase of the radius of the bubble rafts, the core structure parameters η_0 obtained in the P-N theory decreases with the increases with the bubble radius. The dislocation core width of large bubble rafts is narrower than that of small ones. As is well known, the modification of discrete lattice effect is obvious for narrow dislocations. The core structure parameters η obtained in the modified P-N theory also decrease of the bubble radius. It is found that $\Delta\eta = \eta - \eta_0$ are in the small range $2.1 \sim 2.6$ for radius of bubble rafts in the range 0.592 mm ~ 1.682 mm. Thus, $\frac{\Delta\eta}{\eta_0}$ is used to represent the degree of the modification of the discrete lattice effect, and which increases with increase in the bubble radius. As shown in Tab. 1, $\frac{\Delta\eta}{\eta_0} = 91.3\%$ for $R = 1.682$ mm bubble rafts and $\frac{\Delta\eta}{\eta_0} = 51.1\%$ for $R = 0.888$ mm bubble rafts, namely the degree of discrete lattice discrete effect of modification is larger for bigger bubble rafts with narrow dislocations therein. The half core width of dislocations ζ_0 obtained in the P-N theory and ζ achieved in the modified P-N theory, defined as the range of positions within which displacement changed form 0 to $\frac{b}{4}$, are presented in Tab. 1. It is obviously that the discrete lattice effect is important for dislocation core width in bubble rafts, which cannot be neglected.

While the maximum shear stress $\sigma_{\max} = 1.0$ $\left(\text{in units of } \frac{\mu b}{2\pi d}\right)$ without consideration of the position of $\sigma_{\max}$, the core structure parameters are $\eta_0 = 1.0$ and $\eta = 3.4$ for the P-N equation and the modified P-N equation, respectively. $\eta_0 = 1.0$ signifies the classical P-N solution. Foreman's solution is identical with the variational solution if the parameter η is replaced by $\frac{1}{1-c}$ [20]. Therefore, the core structure parameter $\eta = 3.4$ is the same as $c = 0.71$

Table 1. The bubble radius R (in units of mm), the maximum shear stress $\sigma_{\max}$ (in units of $\frac{\mu b}{2\pi d}$, which is taken from Ref. [8]), the core structure parameters η_0 and η, the core width ζ_0 and ζ (in units of b), Peierls stress σ_P (in units of μ).

R	$\sigma_{\max}$	η_0	η	$\Delta\eta$	$\frac{\Delta\eta}{\eta_0}$	ζ_0	ζ	σ_P
1.682	0.728	2.3	4.4	2.1	91.3%	0.79	1.30	4.09×10^{-6}
1.420	0.638	2.7	4.9	2.2	81.4%	0.88	1.42	6.73×10^{-7}
1.332	0.623	2.8	5.0	2.2	78.6%	0.91	1.45	4.68×10^{-7}
1.080	0.513	3.6	5.8	2.2	61.1%	1.10	1.65	2.46×10^{-8}
0.888	0.430	4.5	6.8	2.3	51.1%	1.32	1.90	5.80×10^{-10}

for illustrating the dislocation core structure. While the restoring force law is sinusoidal and the modified P-N dislocation equation is solved with the variational method (following the procedure in Ref. [20]), the parameter c equals to 0.71. The agreement of the results from Foreman's method and variational method shows that the core structure of dislocations in bubble rafts determined here are acceptable. In Fig. 2, the shear stress $\sigma(u)$ for bubble rafts with radius $R = 1.682$ mm and $R = 0.888$ mm are plotted and compared with the previous results. As can be seen, the different values of the core structure parameters η_0 and η give nearly the same shear stress $\sigma(u)$ and the maximum shear stress is the same. The position of the maximum shear stress of the restoring force law in Ref. [8] is deviated from the middle point ($u = 0.25b$), however that does not affect the results discussed here.

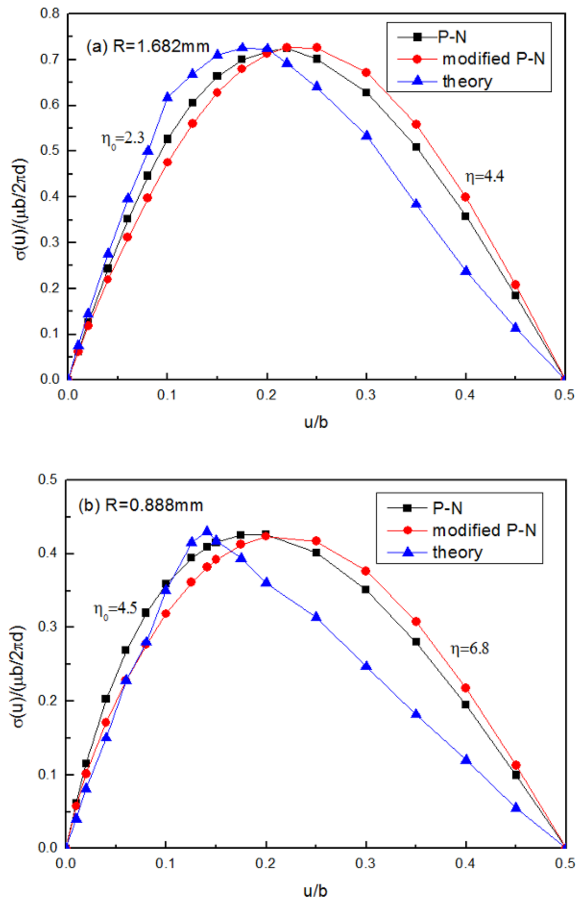

Figure 2. The shear stress $\sigma(u)$ in P-N theory and modified P-N theory comparing with the theoretical restoring force law (which is taken from Ref. [8]), and the core structure parameter η_0 and η is determined.

3. Peierls stress of dislocations in bubble rafts

In the classical P-N theory, the Peierls stress (the minimum applied shear stress moving a dislocation) is calculated by summing the local misfit energy between atoms rows on each side of the glide plane, viz. only the contribution of the misfit energy is considered. However, it has been shown that the elastic strain energy has the same magnitude as the misfit energy. Therefore, the contribution of elastic strain energy should be taken into account and cannot be neglected [20]. The dislocation contains the contribution of misfit energy and elastic strain energy can be expressed as

$$E_{dis}(x_0) = \sum_{n=-\infty}^{n=+\infty} \gamma[u(nb - x_0)] + \frac{1}{2}\sum_{n=-\infty}^{n=+\infty} f[u(nb - x_0)]u(nb - x_0), \tag{5}$$

where x_0 is the position of the dislocation center, the dislocation energy depends on the position of the center of the dislocation x_0. The fist term is the misfit energy $E_{mis}(x_0)$, which results from the atomic interaction across the glide plane. The second term is the elastic strain energy $E_{ela}(x_0)$, which is neglected in the classical P-N model. $\gamma(u)$ and $f(u)$ are the GSF energy and the restoring force law, respectively. By means of Poisson's formula, the misfit energy and the elastic strain energy take the following form

$$E_{mis}(x_0) = \sum_{m=-\infty}^{m=+\infty} \frac{e^{2\pi i m \frac{x_0}{b}}}{2\pi i m} \int_{-\infty}^{+\infty} f(u)\rho(x)e^{2\pi i m \frac{x}{b}}\,dx, \tag{6}$$

$$E_{ela}(x_0) = \sum_{m=-\infty}^{m=+\infty} \frac{e^{2\pi i m \frac{x_0}{b}}}{2b} \int_{-\infty}^{+\infty} f(u)u(x)e^{2\pi i m \frac{x}{b}}\,dx. \tag{7}$$

For bubble rafts, only the restoring force law is known and the GSF energy is unknown. Foreman et al. approximated the Peierls stress by using the cosine-type GSF energy (the corresponding restoring force law is sinusoidal) to calculate the misfit energy [7]. As mentioned before, the restoring force law in bubble rafts deviates from a sinusoidal one. Therefore, the definition of the restoring force $f(u) = -\frac{\partial \gamma(u)}{\partial u}$ and the integration by parts are used while deriving the Eq. (6). The Peierls stress can be obtained from the maximum slope of the dislocation energy

$$\sigma_P = \max\left|\frac{1}{b}\frac{dE_{dis}(x_0)}{dx_0}\right|. \tag{8}$$

After a long and tedious calculation, the Peierls stress still can be written in two parts: σ_P^{mis} and σ_P^{ela}

$$\sigma_P = \sigma_P^{mis} + \sigma_P^{els}, \tag{9}$$

where σ_P^{mis} and σ_P^{ela} indicate the contribution of the misfit energy and the elastic strain energy to the Peierls stress

$$\sigma_P^{mis} = \frac{\kappa_0 b\xi}{96\pi^2\eta^3(1-\nu)}\left[\sigma_{Pa}^{mis} + \sigma_{Pb}^{mis}\right]e^{-\eta\xi}, \tag{10}$$

$$\sigma_P^{ela} = \frac{1}{2\pi^2\eta^2(1-\nu)}\left[\sigma_{Pa}^{ela} + \sigma_{Pb}^{ela}\right]e^{-\eta\xi}, \tag{11}$$

where σ_{Pa}^{mis}, σ_{Pb}^{mis}, σ_{Pa}^{ela} and σ_{Pb}^{ela} are listed in Appendix with $\xi = \frac{2\pi}{\kappa_0 b}$. The Peierls stress is proportional to $e^{-\eta\xi}$, which is similar to the expression of the Peierls stress obtained in the P-N theory for a sinusoidal force law

$$\sigma_P \propto e^{-\frac{2\pi}{\kappa_0 b}}$$

[12]. The new expression of the Peierls stress presented here is not explicitly dependent on a particular form of the restoring force law. Therefore, it is expedient to predict the Peierls stress for dislocations where the core structure parameter is determined. The Peierls stress of dislocations in bubble rafts with different radii is calculated with the new expression. The results are listed Tab. 1. The Peierls stress decreases rapidly with the decrease of the radius of bubble rafts.

4. Conclusions

The core structure and Peierls stress of the dislocations in bubble rafts is investigated within the modified P-N model in which the discrete lattice effect is taken into account. The discrete lattice effect is important for dislocations. The core width obtained in the modified P-N model is much wider than that obtained in the P-N model. The core width of dislocation is increases with the decrease of the bubble radius. The elastic strain energy associated with the discrete effect is considered while calculating the Peierls stress. The new expression presented for the Peierls stress is not explicitly dependent on a particular form of the restoring force law. The Peierls stress is decreases rapidly with decrease of the bubble radius.

Appendix

The calculation of σ_{Pa}^{mis}, σ_{Pb}^{mis}, σ_{Pa}^{ela} and σ_{Pb}^{ela} are long and tedious, and expression for them are given directly as follows

$$\begin{aligned}
\sigma_{Pa}^{mis} =& \beta\kappa_0(1-\nu)\left(3 - 3\eta(4-\xi) + 2\eta^4(3-\xi)\xi^2 + \eta^5\xi^3\right.\\
&\left.+3\eta^2(5-4\xi) + \eta^3\xi\left(15 - 6\xi + \xi^2\right)\right),\\
\sigma_{Pb}^{mis} =& 2\mu\eta^3\left(6 + (\eta-1)\xi(\eta-1)^2\xi^2\right),\\
\sigma_{Pa}^{ela} =& \beta\kappa_0\left(-(6 - 8\eta - 6\nu + 8\eta\nu)\Lambda_1\right.\\
&-(4 - 8\eta - 4\nu + 8\eta\nu)\Lambda_2 + 2(1-\nu)\Lambda_3)\\
&+ \frac{\pi\beta}{12\eta b}(1-\eta)\left(3 + 3\eta(-2+\xi)(1+\eta\xi)\right.\\
&\left.-2\eta^3\xi^3(1-\eta)\right)(1-\nu),\\
\sigma_{Pb}^{ela} =& \mu\left(-4\eta(2-3\eta)\Lambda_1 - 4\eta(4-7\eta)\Lambda_2 + 12\eta^2\Lambda_3 + 4\eta^2\Lambda_4\right)\\
&+ \frac{\pi\mu}{4}(1-\eta)\left(1 + \eta(-3+\xi) - \eta^2(-1+\xi)\xi + \eta^3\xi^3\right)
\end{aligned}$$

with

$$\begin{aligned}
\Lambda_1 =& \frac{\pi}{576}\left(30 + 30\eta\xi + 39\eta^2\xi^2 + 11\eta^3\xi^3\right)\\
&+ \frac{\pi\eta\xi}{96}\left(-3 + 3\eta\xi - \eta^2\xi^2\right)e^{2\eta\xi}\Gamma(0, 2\eta\xi)\\
&- \frac{\pi\eta\xi}{96}\left(3 + 3\eta\xi + \eta^2\xi^2\right)(e_c + \ln 2\eta\xi),\\
\Lambda_2 =& \frac{\pi}{24}\left(1 + \eta\xi + \frac{5}{8}\eta^2\xi^2 - \frac{11}{24}\eta^3\xi^3\right)\\
&- \frac{\pi\eta\xi}{96}\left(3 - 3\eta\xi - 3\eta^2\xi^2\right)e^{2\eta\xi}\Gamma(0, 2\eta\xi)\\
&+ \frac{\pi\eta\xi}{96}\left(-3 - 3\eta\xi + \eta^2\xi^2\right)(e_c + \ln 2\eta\xi),\\
\Lambda_3 =& \frac{\pi}{576}\left(66 + 66\eta\xi - 69\eta^2\xi^2 + 11\eta^3\xi^3\right)\\
&- \frac{\pi\eta\xi}{96}\left(15 + 9\eta\xi + \eta^2\xi^2\right)e^{2\eta\xi}\Gamma(0, 2\eta\xi)\\
&- \frac{\pi\eta\xi}{96}\left(15 - 9\eta\xi + \eta^2\xi^2\right)(e_c + \ln 2\eta\xi),\\
\Lambda_4 =& -\frac{\pi}{576}\left(300 + 300\eta\xi - 123\eta^2\xi^2 + 11\eta^3\xi^3\right)\\
&+ \frac{\pi}{96}\left(48 + 57\eta\xi + 15\eta^2\xi^2 + \eta^3\xi^3\right)e^{2\eta\xi}\Gamma(0, 2\eta\xi)\\
&+ \frac{\pi}{96}\left(48 - 57\eta\xi + 15\eta^2\xi^2 - \eta^3\xi^3\right)(e_c + \ln 2\eta\xi).
\end{aligned}$$

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