Optimizing Radiofrequency Field and Induction Coupling in Slotted Cold Crucibles

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Abstract

Using radiofrequency (rf) for heating and levitation of alloy samples is greatly simplified by a passive element, the slotted cold crucible (similar to Faraday shield for rf plasma ion sources), which if properly designed can shape and concentrate the axial (non static) magnetic field profile. The effect is better represented and verified in 3D simulations (very time consuming) as shown here, even if some simplified 1D and 2D models may help understanding. Boundary conditions at large radius are discussed. Moreover, the sensitivity to important parameters (levitated weight vs frequency and power, sizes of crucible, sample conductivity, radius of sample to skin depth ratio) are demonstrated in a schematized 3D geometry, easily parametrized. Finally complete 3D simulation of a realistic design (adequate for clean alloy melting) are also reported.

1 Introduction

Radiofrequency heating is well established in several applications, including ion source plasma\(^{[1]}\), so that its use for melting alloys (or heating samples) is natural\(^{[2]}\); the Lorentz force on current induced in the sample may (on average) support the sample against gravity, providing levitation for adequate objects and magnetic field B profiles; let us consider cylindrical coordinates \(\psi r z\), with gravity directed towards the negative \(z\). For simplicity let sample be a radius \(R_s\) sphere (or an ellipsoid, see Fig. 1), centered at \(z_s\); all coils have the same axis \(z\) and one only angular frequency \(\omega\), with frequency \(f = \omega/2\pi\) ranging from 1 kHz to 10 MHz as later optimized. Since induced current is mostly in \(\psi\) direction, the support force has a zero on the \(z\) axis, where sample is supported by surface tension and dynamical effects\(^{[2]}\), to be verified in following studies; here we simply compute the total rf power \(P_t\) and the total force \(F_z\) for a given total sample volume \(V_s\), defining the average critical density:

\[
d_a = F_z/(g V_s)\quad d_w = d_a/P_t
\]

(1)

to be compared with \(d_s\) the density of sample; of course \(d_s < d_a\) is a necessary (but not sufficient) condition for levitation, otherwise the sample will fall; in other words, when the critical density per unit power \(d_w\) is calculated, we know that \(P_t > d_s/d_w\) for levitation. We have vector potential \(A \equiv \Re e A_{\psi}(r,z)e^{i\omega t}\); the real part \(\Re\) operator is usually omitted (phasor notation). The rf power is dissipated in the coil, in the crucible (with conductivity \(\sigma_c\)) and in the sample (with conductivity \(\sigma_s\)), mainly dependent from their skin depths

\[
\delta_c = (\mu_0 \sigma_c / 2)^{-1/2} \quad \delta_s = (\mu_0 \sigma_s / 2)^{-1/2}
\]

(2)

When \(\delta_s \ll R_s\) the power loss in sample \(P_s\) is easily estimated by a surface integral

\[
P_s = \frac{1}{2} \int dS Z'_e |H_1|^2 \quad Z_e = (1 + i)/\sigma_c \delta_s = (i \mu_0 \sigma_s / 2)^{1/2}
\]

(3)

where \(Z'_e = \Re Z_e\) with \(Z_e\) the planar surface impedance, \(dS\) is the surface element and \(H_1\) are the tangential components of the magnetic field. Similarly for coils and crucible, with impedance \(Z_c\), which is convenient to keep as low as economically feasible; this implies they are made of copper alloys (with water cooled channels); we define the parameter

\[
M = R_s / \delta_s, \quad \text{so eq. 3 applies for large } M.
\]

For any \(M\), in 3D simulations, power loss \(P_t\) is calculated from applied voltage and currents and also verified by volume integrals.

Figure 1. Sketch of test geometry (not to scale): (a) \(rz\) section (note size definitions); (b) quarter of \(xy\) section (sample omitted); (c) 3D view of coil, sample and a quarter of crucible.
2 The 3D test simulation setup

As shown in Fig. 1, the helical coil of pitch \( p \) with \( N \) complete turns can be approximated with \( N \) rings with conductor radius \( R_w \), average coil radius \( R_c \), provided that[3] each ring has an infinitesimal thin cut to apply a voltage \( V_n \) per turn for current control; due to crucible \( \phi \equiv 0 \) except for coil applied voltage. Since \( \mathbf{E} = -\mathbf{A}_t - \nabla \phi \), the total current density results

\[
j = \sigma \mathbf{E} = -\sigma [i\omega \mathbf{A} + (2\pi r)^{-1} V_n] \tag{4}\]

The current \( I_n \) in each ring \( n \) must equal one common value \( I_c \), so that \( V_n \) must be adjusted until \( I_n = I_c \) (most solvers[5] now include this option; otherwise, \( V_n \) is iteratively adjusted by an user code until \( I_n = I_c \) is satisfied within 0.02% tolerance). The Maxwell equation

\[
\nabla \times \mathbf{H} = j + \mathbf{D}_i, \quad \mathbf{H} = \mu^{-1} \nabla \times \mathbf{A} \tag{5}\]

is discretized using so-called edge elements[4] for \( \mathbf{A} \) (complicate details about gauge fixing and differentiation of \( \mathbf{A} \) are discussed elsewhere [5]). Note that \( \mathbf{D}_i \) is of order \((\omega R_c/c)^2\) and thus usually negligible. At material interfaces, we have the conditions of continuity of \( \mathbf{H}_t \) and of normal component \( B_n \) of the magnetic flux density.

To complete geometry description, the ring assembly height is \( L_a = (N - 1) p + 2R_c \) (the real helical coil length is \( Np + 2R_c \)), while shortest distance between rings is \( p - 2R_c \); in our test case, \( N = 6, p = 0.02 \text{ m} \) and \( R_c = 0.07 \text{ m} \), so that \( L_a \) and \( 2R_c \) are comparable. Crucible outer radius is \( R_1 = 0.06 \text{ m}, \) length \( L_c = 0.12 \text{ m}, \) while inner radius ranges from \( R_3 = 0.02 \) (lower hole) to \( R_2 = 0.04 \text{ m} \) (upper hole); gap seminewidth \( g_s \) is 1 mm. We define a cartesian system Oxz and spherical system \( Op\theta \psi \) related to cylindrical \( Or\psi z \) by \( r^2 = r^2 + z^2 = x^2 + y^2 + z^2 \) and \( z = \rho \cos \theta \) (please note \( \theta \) is the polar angle while \( \psi \) is the azimuth and \( \rho \) the spherical radius). Outer boundary is a large spherical surface \( \rho = R_0 \); in our example \( R_0 = 0.31 \text{ m} \).

It is convenient to simulate only one quarter of geometry, using symmetry at planes \( xy \) and \( yz \); here the boundary condition (bc) is \( B_n = 0 \), that is no field line crosses these surfaces, that is magnetic insulation (for connected boundaries this gives \( \mathbf{A}_t = 0 \)). As to the outer sphere, even for reasonably large \( R_0 \), magnetic insulation is a fair to poor approximation; the seemingly simpler \( H_l = 0 \) (negligible magnetic field) condition is also worst; multiphysics codes now offer the option to add infinite elements around the \( R_0 \) sphere, at the price of computation time. Alternatively, a physically correct boundary condition is the dipole one, see eq. 7, as shown just below. Note that for large \( \rho \) the quadrupole and higher terms are negligible with respect to the dipole term

\[
A_{\psi} = -\frac{\mu_0 m_d}{4\pi} \sin \theta \frac{1}{\rho^2} (1 - ik \rho) e^{ik \rho} \tag{6}\]

with \( k = \omega/c \) and \( m_d \equiv \frac{1}{2} \int x \times j d^3x \), with \( d^3x \) the volume element; the dipole term satisfies the bc:

\[
-\mathbf{n} \times \mathbf{H} = \frac{k_c}{\mu_0 R_0} \mathbf{P} \mathbf{A}, \quad \mathbf{P} = 1 \mathbf{r}^{-1} \begin{bmatrix} -y^2 & xy & 0 \\ xy & -x^2 & 0 \\ 0 & 0 & 0 \end{bmatrix} \tag{7}\]

and \( k_c \equiv (1 - \frac{1}{2} \rho_0^2)/(1 + \frac{1}{2} \rho_0^2) \) with \( k_0 = \omega R_0/c \), as verified by standard calculations. For no crucible case, the dipole moment is \( m_d = \pi N R_c^2 I_c \). Otherwise, let \( z = z_0 \) the middle plane of each ring and \( C_n \) the area of the crucible cut by this plane; in first approximation, the dipole moment \( m_n \) (due to \( n \)-th ring) is reduced as the ratio of this area to whole ring enclosed area \( \pi R_c^2 \). Thus \( m_n = \pi R_c^2 I_c E_n \) with factor \( E_n = 1 - (C_n/\pi R_c^2) \) related the empty space fraction inside ring and \( m_d = \sum m_n \). Moreover the weighted average of ring positions \( z_c = \sum z_0 m_n/m_d \) is computed before simulation, and, coil, crucible, and load are translated by \(-z_c\). After translation \( z_c = 0 \); this coil centering further suppresses non-dipole terms, as verified at simulation end, by a plot of \( H_t \) on the outer sphere.

![Figure 2. Simulated resistance of a pure coil vs. \( N_d \) (ndof), for several mesh styles \( m = 0, \ldots, 7 \), as labeled, with parameters \( h_1, h_2 \) (see text for their definition); theory results without (‘-prox’) and with proximity (‘+prox’) effect are shown as lines; Bu1926 is Ref[6].](Image 336x368 to 529x519)

3 Simulation validation and results

Making a 3D model mesh requests several choices of where to refine the mesh, which should be thinner than \( \delta \), at crucible and coil faces; several mesh styles (numbered with \( m \) in Fig. 2) were compared at \( f = 400 \text{ kHz} \), perhaps with local refinements \( h_1 \) (coil surface element size) and \( h_2 \) (element size of some crucible surface) added to solver standards. The solver normal mesh is \( m = 2 \) (actually very coarse), the finest standard solver mesh is \( m = 1 \), while \( m = 0 \) refines normal mesh on gap surface; other cases add more local refinements to a moderately fine mesh; finally style \( m = 7 \) uses layer elements thinner than \( \delta \) in the coil and the sample. The impedance \( Z_e(c) \) of an rf coil is well-known[6, 7], even if several effect needs to be taken into account, including skin depth and proximity effects. Simulations, when crucible and load conductivities are set to zero, must match result: let \( Z_e(\text{sim}) = \sum V_n/I_c \). The resis-
The near axis field \( B_z(0,0,z) \) (solid line) with maximum at \( z_M \) and plateau at \( z_P \); note also: the crucible outline (dotted line), the field \( B_z \) for \( x = R_1 \) and \( y \ll g_s \) (dashed line), where the six coil turn peaks are visible, and for \( x = R_1 \) and \( y \ll g_s \) (dot-dashed line), where compression at \( z_M \) and corner peaks are visible.

Crucible and coil conductivity were set to \( \sigma_c = 5.8 \times 10^7 \) S/m (cooled copper, plumbing grade) in Fig. 3, showing \( B_z \) on axis for \( I_c = 1800 \) A and \( \sigma_f \) negligible; note the strong asymmetry induced by crucible shaping in an otherwise symmetric coil (no taper); ratio \( \mathcal{R}(z_M, z_P) \) of \( B_z \) at \( z_M \) and \( z_P \) is satisfactorily about 2.5, which increases to 3 when \( B_z \) on the line \( y = 0 \) and \( x = R_1 \) is considered. Indeed the flux \( \Phi^z(z) \equiv \pi B_z r_i^2 \) inside crucible inner radius \( r_i(z) \) would be constant if \( N_{cgs} = 0 \) with \( N_c \) the number of cuts; more precisely, the flux change (leak or increase) rate is

\[
\Phi^z_x = -2 N_{cgs} B_z (r_i^2, 0, z) \quad , \quad r_i^+ = r_i + \varepsilon_i \tag{8}
\]

which is part of an approximate 1D model for \( \Phi^z \) and \( B_z \); here \( \varepsilon_i \) is a small positive length, say \( \varepsilon_i \approx g_s \). This model will give \( \mathcal{R}(z_M, z_P) \approx (r_i(z_P)/r_i(z_M))^{\alpha} \approx 4 \) with \( \alpha = 2 + O(N_{cgs}/R_3) \), from Fig. 4 data we see \( \alpha \approx 1.3 \) for flux leakage. The actual \( \mathcal{L}_c \equiv N_{cgs}/R_3 = 0.1 \) (named leakage parameter, necessarily \( \mathcal{L}_c < \pi \)) here shown is a compromise between trapping flux in the crucible taper and accumulating flux in the \( r_i = R_3 \) part. In Fig. 3, note also the naive estimate \( B_z^{ref} = \mu_0 I_c / p \) and the field on the \( x = R_1 \) line [at square marker in Fig. 1(b)], which shows oscillation due to coil structure and an average lower than \( B_z^{ref} \) by a factor similar to \( f_N \), the well-known Nagaoka factor \( f_N \) [7], roughly \( f_N \approx 1/(1 + 0.9R_c/(Np)) \).

Reported conductivity is about \( \sigma_c = 6 \times 10^5 \) S/m for Ti just above melting point (or \( 10^5 \) S/m for liquid Mo), then it decreases with temperature [8], so range \( \sigma_c = [0.4, 1] \times 10^6 \) S/m is studied here. A \( \sigma_f > 0 \) modifies the \( B_z(z) \) profile, making a valley around \( z_0 \) as shown in Fig. 4; moreover the field phase changes significantly in the sample, as shown by \( B_i^z \) (component in quadrature wrt \( I_c \)). Anyway \( d_a(z) \) as a function of \( z_0 \) seems closely proportional to \( -B_{zz}(z) \) from Fig. 3 data, (no sample) at least for the simulated condition \( f = 21 \) kHz, with an ellipsoidal sample, \( xy \) section radius \( R_x = 0.01 \) m, semi-height \( 0.02 \) m), which is remarkable. Since \( f \) is constant, also \( d_a \) is roughly proportional to Fig. 3 result for \(-B_{zz} \). For stability, the lift must decrease when \( z_0 \) increases, which give the criterion \( B_{zz}(z_0) < 0 \), satisfactorily satisfied in a large interval (including taper of \( r_i \)); for adequate power, an equilibrium \( z_0 \) is then possible. Finally in Fig. 5, with \( z_0 = -17 \) mm fixed, effect of \( R_c \) change and \( \omega \) change is shown; optimal \( d_a \) is reached for \( M \) between 3 and 4 and is roughly proportional to \( \sigma_f^{0.6 \pm 0.1} \).
4 Improved crucible design

Based on the trend observed in the test simulations and on practical consideration, some improvements were made to our reference parameters, see Fig. 1. First, since flux compression increases with sample radius (or when sample to crucible distance \( \equiv R_2 - R_1 \) decreases) a relatively large sample \( R_1 = 15 \) mm was used (actually \( R_1, R_2, R_3 \) and \( p \) have been decreased, respectively to 24.5 mm, 20 mm, 31.5 mm and 11 mm, for prototype construction economy). Second, since the lift strongly depends on fluxline compression in the lower aperture (increasing as \( R_2/R_3 \)), the radius \( R_3 \) was further decreased (to about 5 mm average, with some rounding), which also leaves more space for cooling channels.

![Figure 6](image-url)  
**Figure 6.** The critical density \( d_c \) vs sample center \( z_s \), with \( I_c = 1 \) kA.

![Figure 7](image-url)  
**Figure 7.** The field \( B_z \) along the crucible axis \( z \) for various sample position \( z_s \), for the \( f = 100 \) kHz case.

New geometry considers a larger number of cuts (\( N_c \) from 10 to 12) for better uniformity, with reduced cut width \( 2g_s \leq 0.75 \) mm, so that the leakage parameter \( L_c \approx 0.2 \) still satisfies \( L_c \ll 1 \). We have five or more coil turns, \( N \geq 5 \), and cuts are limited to \( z < z_2 = 64 \) mm, where now \( z = z_3 = 0 \) is the lower crucible face; the upper crucible face is \( z = z_1 = 80 \) mm. Figures 6 and 7 show the quantity of Fig. 4 for the new geometry and parameters; in particular \( I_c = 1 \) kA, \( N_c = 10 \) and \( \sigma_s = 7.4 \times 10^5 \) S/m; moreover \( N = 6 \) and coil wire radius \( R_w = 4 \) mm. The external boundary conditions is made with an infinite element. The magnetic field and the force obtained on the crucible has been studied as function of the sample position \( z_s \); considering geometry constraint and large CPU-time requested for each simulation, scan of \( z_s \) was limited to the \([32,50] \) mm inter-

val. As manifest in Fig. 6 result for \( d_s \), only the \( z_s \in [32,36] \) mm range is stable [that is, \( d_s(z_s) \) decreasing, but positive], which is reasonable, since this range corresponds to larger \( d_s \), achieved only when the spherical sample is very near to the crucible bottom. When the sample ball is in the middle of the crucible, lift force and \( d_s \) become zero or negative. Note also that \( B_z \) is much larger below sample than it is over sample (see fig. 7), due to the realistic absence of cuts over the \( z = z_2 \) planes. The maximum of magnetic field is very near to the crucible bottom. Note the perspective advantage that sample is mainly heated in its lower part, so improving convection inside sample.

This demonstrates that crucible shape can be reliably optimized even under realistic conditions, with traceable effects of design modifications. The contactless heating of alloys (in vacuum or controlled atmosphere) will allow a host of technological applications; also rf field enhancement is remarkable.

References


