OPEN ACCESS
IOP Publishing
Superconductor Science and Technology
Supercond. Sci. Technol. **38** (2025) 049501 (3pp)
https://doi.org/10.1088/1361-6668/adbce1

Corrigendum: *In-situ* synchrotron x-ray photoelectron spectroscopy study of medium-temperature baking of niobium for SRF application (2024 *Supercond. Sci. Technol.* 37 075007)

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Received 6 February 2025
Accepted for publication 5 March 2025
Published 20 March 2025

Abstract

Upon reviewing the published version of our work, we identified misprints in the equations, which are corrected here. Additionally, we re-evaluated the oxygen concentration depth profiles. This re-evaluation does not affect the validity of the paper's statements or conclusions.

1. Misprints in equations

Typographical errors occurred in equations (3) and (4) of the original paper. The correct forms of these equations are as follows:

$$C = \frac{1}{\sqrt{\pi D}} \int_0^t \mathrm{e}^{-x^2/(4Dt)} \frac{\varphi(t)\,\mathrm{d}t}{\sqrt{t}}, \tag{3}$$

$$C = 2\nu\sqrt{\frac{t}{\pi D}}\mathrm{e}^{-x^2/(4Dt)} - \frac{\nu x}{D}\mathrm{erfc}\frac{x}{2\sqrt{Dt}}. \tag{4}$$

However, the calculations presented in the paper in figure 12 were performed using equation (4), which was free of typographical errors, and are therefore correct.

2. Additional analysis of oxygen concentration profiles

In this analysis, we re-evaluated the oxygen concentration depth profiles, despite this does not affect the statements or conclusions of the paper. For simplicity, the paper assumed that the oxide dissolution rate does not depend on time, i.e. $\varphi(t) = \nu$, a constant. Thus, equation (4) was applied with $\nu_1 = k_1 C_0$ and $\nu_2 = k_2 C_0^2$ for first- and second-order reactions, respectively. However, this assumption does not hold

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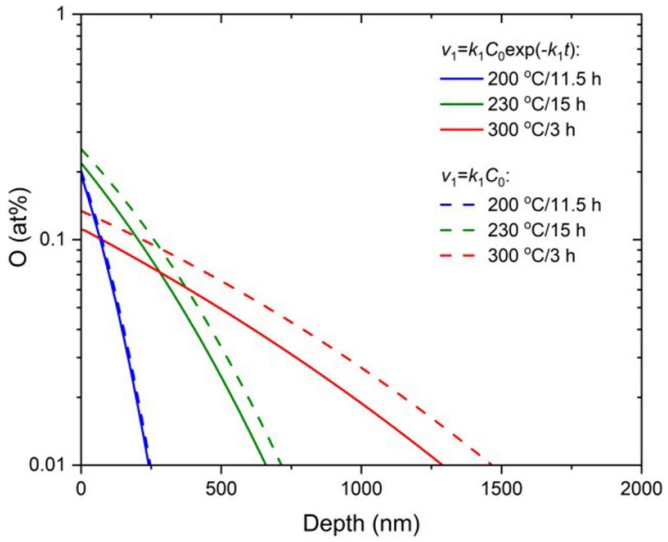

Figure 1. Comparison of calculated oxygen concentration profiles in niobium during annealing at 200 °C–300 °C for $\varphi(t) = \nu = k_1 C_0$ (dashed lines, from equation (4), as in figure 12 of the paper) and $\varphi(t) = k_1 C = k_1 C_0 \exp(-k_1 t)$ (solid lines, from equation (3)) assuming a first-order reaction. Oxygen atoms evolving from the oxide are considered with $C_0 = 142$, excluding near-surface interstitials.

in practice, as the oxide dissolution rate is concentration-dependent, and oxygen concentration varies over time. Consequently, equation (3) must be used. For first- and second-order reactions, the rates are described as:

$$\nu_1 = k_1 C = k_1 C_0 \exp(-k_1 t), \qquad (*)$$

$$\nu_2 = 2k_2 C^2 = \frac{2k_2}{\left(2k_2 t + \frac{1}{C_0}\right)^2}, \qquad (**)$$

where factor of 2 in (**) accounts for the simultaneous involvement of two oxygen atoms in the reduction of Nb_2O_5.

Figure 1 compares oxygen concentration profiles in niobium during annealing at 200 °C–300 °C, calculated using the first (as in the paper) and second approaches. For these calculations, oxygen atoms evolving from the oxide were considered with the average initial concentration within the XPS information depth, $C_0 = 142$, while near-surface interstitial oxygen was neglected.

The previous assumption resulted in a slightly higher integral of diffused oxygen species—up to 20% greater at 230 °C/15 h—compared to the values obtained using the second approach. To validate our earlier assumption, we repeated the calculations with the exact initial oxygen concentration for each sample (see the table).

It should be noted that comparing calculation results with XPS experimental data, especially at temperatures

Table. Number of oxygen atoms (per 100 Nb atoms) diffused into the Nb surface layer during native oxide reduction at specific baking parameters. Calculations used the exact initial oxygen concentration C_0 within the XPS information depth.

Treatment	XPS data	$\nu_1 = k_1 C_0$	$\nu_1 = k_1 C$	$\nu_2 = 2k_2 C^2$
200 °C/11.5 h ($C_0 = 146$)	16	20.0	18.7	21.7
230 °C/15 h ($C_0 = 149$)	54	68.4	55.1	64.6
300 °C/3 h ($C_0 = 135$)	103	79.0	59.9	78.7

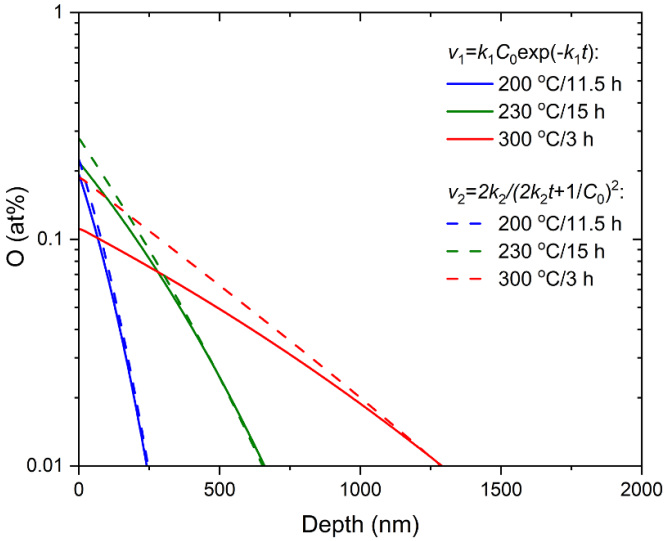

Figure 2. Comparison of calculated oxygen concentration profiles in niobium during annealing at 200 °C–300 °C for $\nu_1 = k_1 C_0 \exp(-k_1 t)$ (solid lines) and $\nu_2 = 2k_2/(2k_2 t + 1/C_0)^2$ (dashed lines), corresponding to first- and second-order reactions.

$\geqslant$300 °C, is not straightforward. The diffusion process during temperature ramping, which is not accounted for in the presented model, becomes significant at higher temperatures.

Figure 2 presents the results of calculations using equation (3) for first- and second-order reactions under the second approach. The oxide dissolution rates are described by equations (*) and (**).

The second-order reaction rate constant is estimated as $k_2 = 8.17 \exp\left(\frac{-79.41\text{kJ/mol}}{RT}\right)$. The total number of diffused oxygen atoms is presented in the table. Similar to the results presented in figure 12 of the paper, ν_2 provides more oxygen atoms dissolved in niobium compared to ν_1.

The total number of diffused atoms shows slightly better agreement with experimental XPS data for the second approach (i.e. $\nu_1 = k_1 C_0 \exp(-k_1 t)$) at temperatures of

200 °C–230 °C, assuming a first-order reaction. At these temperatures, the first-order reaction aligns more closely with experimental data compared to the second-order reaction, consistent with the conclusions of the paper. For a more rigorous evaluation, the diffusion process during the temperature ramping must be incorporated into the model. Additionally, estimating the kinetics of individual reduction steps of the oxide-reduction process might be necessary.

In summary, the re-evaluation of oxygen concentration profiles presented here does not contradict the statements or conclusions of the paper.